Research Program

Nuclear Waste

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The role of ESD's Nuclear Waste Program (NWP) is to assist the U.S. Department of Energy, the United States, and other countries in solving the problem of the safe disposal of high-level radioactive waste—by means of high-quality scientific analyses and technology development. The major portion of this program involves investigating the feasibility and potential of the Yucca Mountain site in Nevada for permanent storage of high-level nuclear waste. The NWP has also collaborated on nuclear-waste disposal issues with such countries as Japan, Switzerland, Sweden, China, Romania, and others.

The Yucca Mountain site is located about 120 km northwest of Las Vegas in a semi-arid region. The proposed repository will be located about 350 m below ground surface within a thick unsaturated zone (UZ). Subsurface rocks at Yucca Mountain consist primarily of fractured volcanic tuffs that vary in degree of welding. To date, a total of about 60 deep surface boreholes have been drilled in the area. In 1996, an 8 km long underground tunnel, the Exploratory Studies Facility (ESF), was completed at Yucca Mountain to facilitate more extensive subsurface testing.

NWP's work at Yucca Mountain consists of solving many problems related to multiphase, nonisothermal flow and transport through the UZ. Some of the key questions addressed by NWP scientists include:

- How much water percolates through the UZ to the repository at Yucca Mountain?
- What fraction of the water flows in fractures and what fraction flows through the rock matrix blocks?
- How much of this water will seep into the emplacement drifts (tunnels)?
- How will radionuclides migrate from the repository to the water table?
- How will coupled TH (thermal-hydrological), THC (thermal-hydrological-chemical) and THM (thermal-hydrological-mechanical) processes affect flow and transport?

To address these questions, the NWP is organized into the Ambient Testing, Thermal Testing, and Modeling groups, with support from geophysical studies.

AMBIENT TESTING GROUP

The Ambient Testing group investigates how water flows through the mountain and how much of this water will seep into the emplacement drifts. This group has performed various tests within the ESF, including fracture-matrix interaction tests, drift-to-drift tests, the Paintbrush unit test (PTn test), and niche (short drift) testing. Fracture-matrix interaction tests are relatively small-scale tests (i.e., covering a few meters) that focus on the components of water flow in fractures and matrix blocks and on the interaction between the two continua. The drift-to-drift tests address the same issues, but on a much larger spatial scale (10–20 m). The test in the Paintbrush unit, which is an unwelded tuff unit, addresses issues of episodic flow, effects of faults and large-scale features, and lateral continuity of flow and transport. This mostly unfractured unit, directly above the potential repository, is key to dispersing fracture flow from the fractured units above it, and buffering the transient behavior of episodic flow. The niche studies address perhaps the most crucial problem of Yucca Mountain, i.e., determining the fraction of water that will flow into the emplacement drifts. The niche studies are carried out by introducing water into boreholes above the drift opening and measuring what fraction actually seeps into the opening.

THERMAL TESTING GROUP

The Thermal Testing group works in collaboration with other national laboratories to evaluate the effects of heat on thermodynamic conditions, fluid flow and transport, and permanent property changes in the fractured tuff at and near the emplacement drifts. The Yucca Mountain Project has completed the first *in situ* heater test, called the Single Heater Test. The project is now conducting a large-scale heater test in a 50 m long drift. This second test, called the Drift Scale Test (DST), is intended to resemble the actual conditions that would exist when the high-level radioactive waste is placed in the emplacement drifts. NWP's roles in the heater tests are to characterize the heater-test rock block (area) prior to testing; to monitor potential changes in fracture and matrix saturations through air injections, tracer testing, and ground-penetrating radar measurements; and to perform predictive TH, THC, and THM calculations.

The initial characterizations of the heater test areas were performed with air-injection tests that yield the 3D permeability structure of the fracture network. Continued air-injection testing during heating yielded changes that can be attributed to changes in fracture saturations or mechanical effects. Crosshole radar tomography has also yielded very promising results regarding change in global saturations of the system caused by heating. Laboratory scientists are also involved with measurements of the isotopic compositions of gases and condensate water collected in instrumented boreholes. Detailed 3D TH, THC, and THM calculations were used to predict the behavior of the tests.

MODELING GROUP

Berkeley Lab has the primary responsibility for the development of the UZ Flow and Transport Model. This is a comprehensive, 3D, dual-permeability numerical model that represents the entire UZ at and near Yucca Mountain. The model is intended to integrate, within a single computational framework, all of the relevant geological, hydrological, geochemical, and other observations that have been made at the surface, in boreholes, and in tunnels at Yucca Mountain. The model is calibrated against pneumatic moisture tension, matrix potential, temperature, geochemical, perched water, and other data from the UZ. The model is then used to predict all of these variables in new boreholes and new drifts to be drilled. The degree of agreement between model predictions and subsequent field observations indicates the reliability of the model, and provides guidance as to what additional data need to be collected and incorporated.

A very important submodel of the UZ model is the seepage model, which is on a tens-of-meters scale, versus the UZ model's hundreds-of-thousands-of-meters scale. The seepage model, similar to the UZ model, predicts the results of the niche tests, which are subsequently modified to match the actual observations. Another submodel of the UZ model is the coupled-process THC model, calibrated using the heater test data and used to estimate the chemistry of water and gas entering the drifts. All these models—the UZ model, the seepage model, and the THC model—are key to the Total System Performance Assessment of Yucca Mountain, since performance of the potential repository is only as reliable as these underlying key models.

FUNDING

The Nuclear Waste Program's Yucca Mountain Project research is supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and Berkeley Lab. The support is provided to Berkeley Lab through U.S. Department of Energy Contract No. DE-AC03-76SF00098.

Evaluation of Seepage During the Thermal Period at Yucca Mountain

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RESEARCH OBJECTIVES

Predicting the amount of water that may seep into waste emplacement tunnels (drifts) is essential for assessing the performance of the geologic nuclear waste repository at Yucca Mountain, Nevada. At ambient temperatures, seepage from the unsaturated fractured tuff into the drifts is reduced by the capillary barrier behavior at the rock-drift interface. In addition, the fractured rock in the drift vicinity will be heated to maximum temperatures of more than 130°C, caused by the radioactive decay of the nuclear waste, and water percolating down towards the repository will be subject to vigorous boiling during the first several hundred years following waste emplacement. Thus, the superheated fractured rock forms a vaporization barrier that may further limit the potential for seepage. To study the impact of the drift-scale thermal-hydrological (TH) perturbations, a TOUGH2 simulation model was developed for the prediction of "thermal seepage" (i.e., seepage during the time that flow is perturbed due to heating).

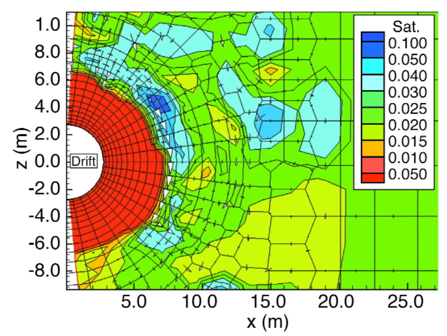

Figure 1. Fracture saturation and liquid flux vectors for a selected simulation case at 100 years of heating

APPROACH

The future TH conditions in the vicinity of waste emplacement drifts at Yucca Mountain are evaluated with a heterogeneous dual-permeability process model. The conceptual framework for describing the TH processes is based on models that accurately represent the thermal response of large *in situ* heater tests. The specific simulation framework for seepage is consistent with the modeling method employed in ambient seepage studies, which was developed based on model comparisons with liquid-release seepage testing. The key elements in this method—small-scale fracture permeability heterogeneity, relatively weak capillary strength, and the effect of discrete fractures at the drift wall—have all been included in the thermal seepage model. Several simulation cases are performed that cover the expected range of TH conditions at Yucca Mountain. Transient seepage rates during the period of enhanced temperatures are directly calculated from the model and compared to the respective seepage rates at ambient conditions.

ACCOMPLISHMENTS

Simulation results demonstrate that the thermal perturbation of the flow field—giving rise to increased downward flux from the condensation zone towards the drifts—is strongest during the first few hundred years after waste emplacement, corresponding to the period when rock temperature is highest and the vaporization barrier is most effective (Birkholzer et al., 2003). Even for high percolation fluxes into the model domain, and strong flow channeling as a result of fracture heterogeneity, water is not predicted to penetrate far into the superheated rock during the time that rock temperature is above boiling, and model results show no seepage (Figure 1). At the time when temperature has returned to below-boiling conditions and fractures start rewetting at the drift, the capillary barrier at the drift wall continues to reduce (or prevent) water seepage into the drift. Seepage is predicted to occur for such simulation cases that feature strongly heterogeneous fracture permeability fields, weak fracture capillary strength in the drift vicinity, and high percolation fluxes. In these cases, water starts to seep several hundred to a few thousand years after the rock temperature has returned to below boiling, the delay caused by the slow saturation buildup in fractures. Seepage amounts increase with time and asymptotically approach seepage rates estimated for long-term ambient conditions.

SIGNIFICANCE OF FINDINGS

The model results consistently demonstrate that (1) seepage does not occur under above-boiling conditions near the drifts, and (2) seepage under below-boiling conditions does not exceed the amount of ambient seepage. These findings are very important for the performance of the nuclear waste repository; they are currently being implemented into the performance assessment supporting the license application process.

RELATED PUBLICATION

Birkholzer, J., S. Mukhopadhyay, and Y.W. Tsang, Modeling water seepage into heated waste emplacement drifts at Yucca Mountain. Proceedings of the TOUGH Symposium 2003, Berkeley, California, May 12–14, 2003.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and the Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab). The support is provided to Berkeley Lab through the U.S. Department of Energy Contract No. DE-AC03-76SF00098.

Systematic Hydrological Characterization of the Topopah Spring Lower Lithophysal Unit

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RESEARCH OBJECTIVES

Over 80% of the proposed repository for the permanent disposal of high-level radioactive nuclear waste will be situated in the lower lithophysal unit of the Topopah Spring welded tuff, Yucca Mountain, Nevada. Within the Exploratory Studies Facility at Yucca Mountain, a 5 m diameter drift (tunnel), called the East-West Cross Drift, traverses this lower lithophysal unit. The welded tuff is intersected by many submeter fractures and interspersed with lithophysal cavities ranging from 15 to 100 cm in diameter. The size and spacing of both these features (fractures and cavities) varies appreciably. This indicates that hydrological characteristics at one particular location may not be representative of the entire lower lithophysal unit. Therefore, systematic testing at regular intervals, unbiased by the knowledge of specific features, is in progress, with the objective of gaining a greater understanding of the hydrological characteristics and associated heterogeneity of this potential repository unit.

APPROACH

Liquid-release (seepage) tests determine the ability of the open drift to act as a capillary barrier that diverts water around itself. Seepage into drifts increases the potential for corrosion of waste canisters and subsequent release of radionuclides. Seepage tests through this highly heterogeneous rock are being performed every 30 m along an 800 m stretch of the 5 m diameter drift. Water is released steadily into a series of 20 m boreholes drilled upward at a 15° angle along the drift crown. Water that then seeps through the rock is measured by a drip capture system, and evaporation area is estimated using time-lapse photography. Seepage and evaporation are subtracted from the water released to determine how much water has been diverted.

Figure 1 shows a series of time-lapse photos taken of the drift crown as water from a test seeps through. These photos were taken about 6 days apart and show a gradual decrease in the rate of wetting. The photos show the evaporation pan with its white umbrella, which prevents seepage from accidentally filling the pan. The wire mesh (also shown) has a 7.5 cm spacing, which is used to estimate the size of the wet patch. Multiplying this size by the flux from the pan yields the amount of evaporation from the crown. The photos also help determine when the first seep occurs after initiation of water release and how the flow first intersects the drift, whether it be by fractures, through cavities, or in the matrix itself. In addition, these photos help pinpoint whether a threshold water-release-rate value exists, below which no water enters the drift.

ACCOMPLISHMENTS AND SIGNIFICANCE OF FINDINGS

Testing has progressed through the fifth of the series of boreholes along the drift. As the systematic hydrological testing progresses, a catalogue of flow characteristics for the drift is being developed. Not only can the various flow characteristics themselves be logged, but the distances for which they persist along the drift can now also be measured. Length scales from 1 to 23 m, with flow characteristics up to 100% impermeability and 100% diversion, have now become apparent, because of the expansive coverage of drift that can be tested with the systematic approach.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and the Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab). The support is provided to Berkeley Lab through the U.S. Department of Energy Contract No. DE-AC03-76SF00098.

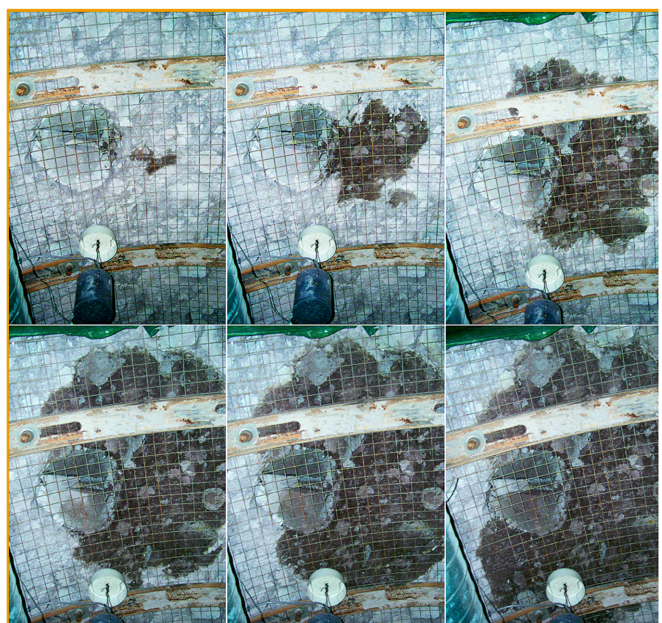

Figure 1. Time-lapse photos of the drift crown under a section of borehole being tested

Investigating How the Multiscale Heterogeneity of Hydrogeologic Properties Affects Flow and Transport at Yucca Mountain, Nevada

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RESEARCH OBJECTIVES

Much of the exposed rock within the underground tunnels at the proposed repository site for disposal of high-level radioactive nuclear waste at Yucca Mountain, Nevada, has been mapped for fractures and cavities. It is thought that such features (the fractures and cavities) would be the most likely pathways for possible hydrological flow. Yet surface feature mapping gives very little indication as to the capability of these features to transmit fluids. An ongoing effort to dynamically "map" potential hydrological features of this type, using pneumatic testing at the Yucca Mountain Exploratory Studies Facility (ESF), has been under way as part of the systematic testing program there. Systematic testing at regular intervals, the choice of which is unbiased by previous knowledge of specific features (such as large fractures or an extra abundance of fractures/cavities), is in progress. This type of testing is crucial for understanding the overall hydrological characteristics and associated heterogeneity of the proposed repository units.

APPROACH

Pre-existing 4 m boreholes, drilled at regular intervals every 5 to 10 m along a 500 m "rib" (wall) of the ESF Main Drift, facilitate a series of pneumatic tests utilizing a borehole packer. Using this packer with pneumatic flow control and pressure measurement equipment enables an air-permeability profile to be developed for each of these boreholes. The spatial resolution of these profiles can be adjusted from the length of the whole borehole down to 0.33 m, allowing different scales of features inside the holes to be measured for air permeability. A statistical understanding of the size of impermeable blocks within the holes and of the frequency and spacing of high-flow features is being developed.

ACCOMPLISHMENTS AND SIGNIFICANCE OF FINDINGS

Testing has progressed through 29 of the series of boreholes. Figure 1 shows the permeability profiles at the 0.33 m resolution in the 29 boreholes along a 230 m section of the drift. There is one borehole longer than the others that is thought to intersect the Sundance Fault of Yucca Mountain. A higher permeability at that location (caused by the fault) may account for the higher peak in the profile seen towards the end of that borehole. That some boreholes have extremely low permeability near the rib is somewhat counterintuitive, when considering that the atmospheric boundary at the rib might bias the measurement to a higher value. The presence of the drift itself, however, may cause existing features, particularly if near-horizontal, to close under load, lowering their permeability. As the systematic pneumatic testing progresses, a catalogue of flow characteristics for a growing length of drift is being developed in two dimensions, spanning a range of scales from the 0.33 m interval length, to borehole scale, to drift scale (obtained from borehole-to-borehole comparisons).

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and the Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab). The support is provided to Berkeley Lab through the U.S. Department of Energy Contract No. E-AC03-76SF00098.

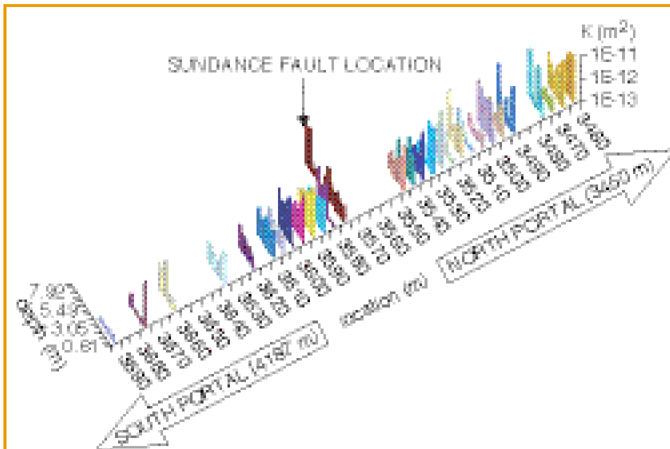

Figure 1. The section of the ESF Main Drift that has been pneumatically profiled

Geothermal Systems as Natural Analogues for Yucca Mountain Coupled Processes

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RESEARCH OBJECTIVES

Geothermal systems provide an ideal opportunity for examining the long-term effects of coupled thermal-hydrological-chemical (THC) processes expected for the proposed radioactive waste repository at Yucca Mountain, Nevada. Active and fossil geothermal systems provide important insights into the consequences of processes such as boiling, condensation, fluid mixing, and water-rock interaction associated with fluid flow in matrix and fractures, and can be used to test coupled-process models. Geothermal systems also allow observation of the effects of processes over much larger volumes and longer time scales than would be possible in laboratory or field experiments. The objective of this study is to evaluate potential changes in fluid flow resulting from the thermal impacts of storing high-level radioactive waste in fractured ash flow tuffs through characterization of the effects of water-rock interaction in geothermal systems.

APPROACH

An extensive literature review was performed to identify well-characterized examples of THC processes in active and fossil geothermal systems. Special attention was given to processes such as heat and fluid flow, chemical transport, boiling and dryout, condensation and mineral dissolution, and mineral alteration and precipitation. In addition, a detailed examination of core samples from the Yellowstone geothermal system was conducted to evaluate the effects of lithology and hydrothermal alteration on porosity and permeability.

ACCOMPLISHMENTS

The review identified key THC processes in geothermal systems and evaluated their relevance to Yucca Mountain. Fluid flow in low-permeability rocks (such as the welded tuffs found at Yucca Mountain) occurs predominantly in fractures. Precipitation of minerals can be triggered by boiling, water-rock interaction, heating and cooling of fluids, and fluid mixing. Mineral solubilities, reaction-rate kinetics, and the flux, chemistry, and temperature of circulating fluids control the rates and volumes of mineralization. Mineral precipitation (typically silica, clays, zeolites, anhydrite, and calcite) occurring within fracture flow pathways can form effective permeability barriers. Self-sealing zones observed in core samples in the Yellowstone geothermal system appear to have resulted from boiling events that led to the development of supersaturated fluids (Figure 1).

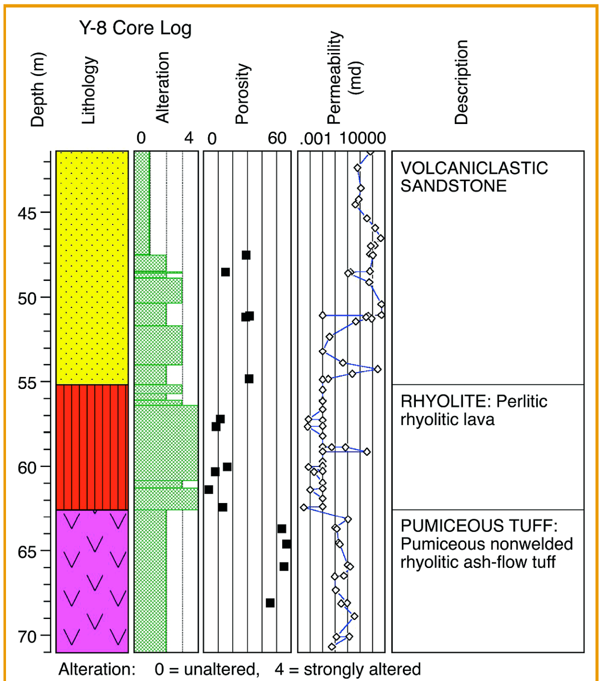

Figure 1. Simplified log of the geology, porosity, and matrix permeability of the Y-8 Yellowstone core. Silicification in the lower portion of the volcaniclastic sandstone unit has resulted in reductions in porosity and permeability, thereby forming an effective seal to the underlying convecting geothermal reservoir.

SIGNIFICANCE OF FINDINGS

Effects of THC processes such as boiling, condensation, dissolution, and precipitation for Yucca Mountain's higher-temperature operating mode will be most significant in the near-field environment (near the proposed repository). However, unsaturated conditions, lower temperatures, and the much lower fluid flow rates predicted for the Yucca Mountain system (in comparison to geothermal systems) should result in less extensive water-rock interaction than is observed in geothermal systems. Current THC models for Yucca Mountain predict that while both amorphous silica and calcite will precipitate in the near-field environment, significant fracture sealing is unlikely.

RELATED PUBLICATIONS

Simmons, A.M., Natural Analogue Synthesis Report. Report TDR-NBS-GS-000027 REV00 ICN 02, Bechtel SAIC Company, Las Vegas, Nevada, 2002.

Dobson, P.F., T.J. Kneafsey, J. Hulen, and A. Simmons, Porosity, permeability, and fluid flow in the Yellowstone geothermal system, Wyoming. J. Volcanol. Geotherm. Res., 123, 313–324, 2003.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and the Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab). The support is provided to Berkeley Lab through the U.S. Department of Energy Contract No. DE-AC03-76SF00098.

Development of Numerical Grids for Unsaturated Zone Flow and Transport Modeling

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RESEARCH OBJECTIVES

Numerical grid generation is an integral part of the development of numerical models used for simulating unsaturated zone (UZ) flow and transport at Yucca Mountain. Previous studies at Yucca Mountain have generated detailed information on the geologic and hydrological properties of the UZ. Information on the stratigraphy, orientation, and location of faults, presence of vitric and zeolitic subunits, hydrological properties of the different hydrogeologic units, the location of the water table, and the design and location of proposed repository drifts can be used to develop complex 3-D numerical grids. The objective of this work is to construct numerical grids that provide the necessary resolution for subsequent UZ hydrological-property and flow calibration and mountain-scale flow and transport simulations for the Yucca Mountain system.

APPROACH

Numerical grid generation is an iterative process that must achieve a proper balance between desired numerical accuracy (requiring more gridblocks) and short computational time (requiring fewer gridblocks). Fault and stratigraphic contact data obtained from the Yucca Mountain Geologic Framework Model were used in conjunction with hydrogeologic unit definitions to form the basis for the development of numerical grids. Other key input data included the location of calibration boreholes, the proposed repository layout, the water table surface (which forms the lower boundary of the UZ), and the location of zeolitic and vitric tuffs within the Calico Hills nonwelded units. These data were used as input for the WinGridder software package to develop 1-D, 2-D, and 3-D numerical grids (Figure 1). The resulting grids were checked using visual inspection and test simulations to verify the accuracy of the mesh and gridblock connections. Fracture data were used along with the program 2kgrid8.for to transform the effective-continuum model 3-D grid into the dual-permeability 3-D numerical grid required for conducting flow and transport models in heterogeneous, fractured rocks.

ACCOMPLISHMENTS

A revised set of 1-D, 2-D, and 3-D numerical grids was generated for use in numerical modeling of UZ flow and transport at Yucca Mountain. These grids incorporated changes made to the Yucca Mountain Geologic Framework Model, the UZ Model area boundaries, the position of the water table, the proposed repository design, and the location of vitric and zeolitic subunits in the Calico Hills nonwelded tuffs. The new grids also contained enhanced vertical resolution in selected units to better resolve processes such as lateral flow.

SIGNIFICANCE OF FINDINGS

The resulting numerical grids have been used for calibration of hydrogeologic unit properties and flow fields, testing of conceptual models of UZ flow and transport, and simulation of mountain-scale flow and transport behavior for the Yucca Mountain system under a variety of climatic and thermal-loading conditions.

RELATED PUBLICATION

Dobson, P.F., L. Pan, and R. Hedegaard, Development of numerical grids for UZ flow and transport modeling. ANL-NBS-HS-0000015 REV01, BSC, Las Vegas, Nevada, 2003.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and the Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab). The support is provided to Berkeley Lab through the U.S. Department of Energy Contract No. DE-AC03-76SF00098.

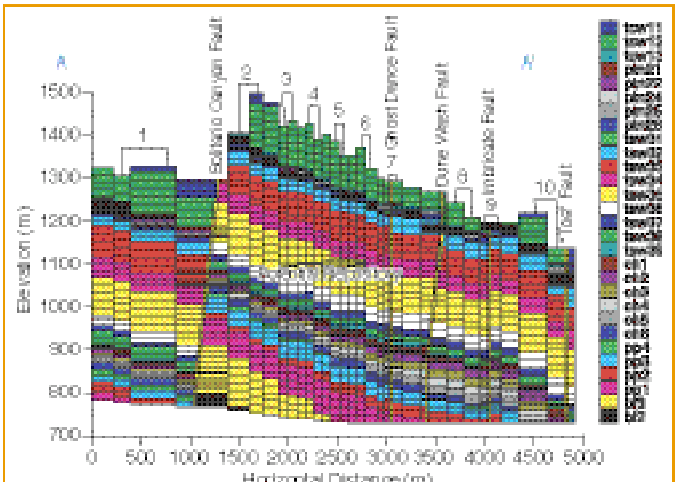

Figure 1. East-west cross section from the UZ Model Grid. Model layers represent hydrogeologic units derived from the Yucca Mountain Geologic Framework Model. Numbered column pairs were used to compare contact elevations obtained from the UZ Model and the Geologic Framework Model.

Scaling and Hierarchy of Models for Flow Processes in Unsaturated Fractured Rock

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RESEARCH OBJECTIVE

The goal of this research is to investigate whether a hierarchy of scales is needed to conduct measurements and develop models for an accurate description of the spatial-temporal behavior of flow and transport processes in unsaturated fractured rock.

APPROACH

The alternative approach to volume-averaging and scaling in unsaturated fractured rock is to use a hierarchy of scales. This approach is based on a system structure, i.e., the classification of a graded (ranked) series of system parts (subsystems). Each subsystem is dominant over those below it and dependent on those above it.

The concept of a hierarchy of scales in unsaturated fractured rock involves the following scales: *elemental*—for laboratory cores or a single fracture at a field site; *small scale* (approximately 0.1–1 m^2)—for a single fracture, including fracture-matrix interaction, film flow, and dripping water phenomena; *intermediate scale* (approximately 10–100 m^2)—for flow in the fracture network on a field scale, and *large scale*—for the fracture and fault network flow. Each of these scales should be investigated on a minimum of three hierarchical levels. For the level of interest, called Level 0, a hierarchy should include at least one hierarchical level above it, called Level +1, and at least one hierarchical level below it, called Level -1. The low-frequency behavior at Level +1 constrains the higher-frequency dynamics of Level 0 and thus determines the system boundary condition, constraining the system behavior over time. Because small-scale intrafracture flow processes are neither physically nor geometrically analogous to large-scale fracture-network processes, different conceptual approaches are required for modeling at different scales.

ACCOMPLISHMENTS

Figure 1 presents an example of a hierarchy of scales for flow processes in fractured tuff at the Yucca Mountain site. If Level 0 investigations are conducted to develop an intermediate-scale model (e.g., flow and transport processes in a fracture network around a tunnel, lateral flow at the interface between the Tiva Canyon and Paintbrush (PTn) hydrogeologic units, dispersion in the PTn unit, and a perched-water zone at the Topopah Spring and Calico Hill interface), Level -1 investigations include the study of small-scale processes taking place in small fractures and lithophysal zones (e.g., seepage, evaporation caused by tunnel ventilation, and intrafracture fingering). Level +1 investigations should be used to assign boundary conditions for the whole TSw unit. We have found that a trace length of 2 m represents a critical fracture length separating small and intermediate scales. A length of 10 m represents a critical fracture length separating intermediate and large scales.

SIGNIFICANCE OF FINDINGS

The concept of a hierarchy of scales and models will improve predictions of both water seepage and chemical transport through unsaturated fractured rocks at different scales, and reduce uncertainty in predictions of such processes.

RELATED PUBLICATION

Faybishenko, B., G.S. Bodvarsson, P.A. Witherspoon, and J. Hinds, Scaling and hierarchy of models for flow processes in unsaturated fractured rock. In: Scaling Methods in Soil Physics (Y.A. Pachepsky, D.E. Radcliffe and H. M. Selim, eds.), pp. 373–417, CRC Press, LLC, 2003.

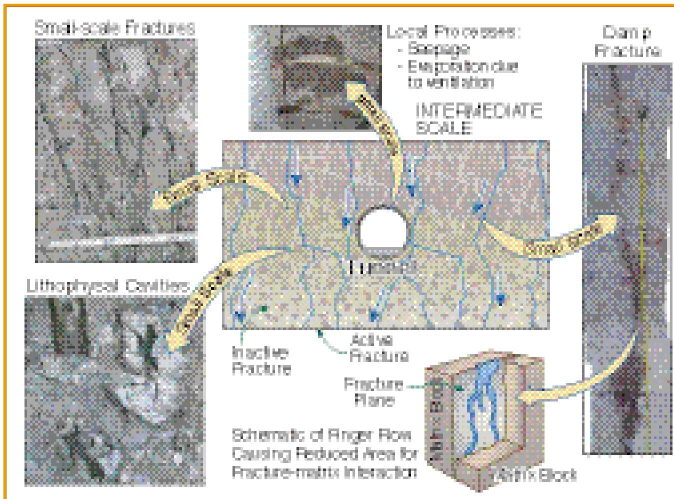

Figure 1. A hierarchy of scales for flow processes in fractured tuff at Yucca Mountain

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and the Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab). The support is provided to Berkeley Lab through the U.S. Department of Energy Contract No. DE-AC03-76SF00098. This work was also supported by the Director, Office of Science, Office of Basic Energy Sciences, of the Environmental Management Science Program of the U.S. Department of Energy, also under Contract No. DE-AC03-76SF00098.

Evaporation from a Seepage Face

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RESEARCH OBJECTIVES

Dripping of water into waste emplacement drifts may critically affect the integrity of waste packages and the mobilization of radionuclides. To characterize seepage from fractured rocks, we release water from boreholes drilled above an underground opening, and collect it as it drips into the cavity. These seepage data are often influenced by evaporation effects caused by drift ventilation.

The objectives of this research are (1) to understand the evaporation mechanism at a rock surface, (2) to study the coupling between near-surface flow in fractured rock and evaporation, (3) to examine the effect of evaporation on seepage, (4) to develop effective simulation capabilities for unsaturated flow and seepage under evaporative conditions, (5) to analyze evaporation and liquid-release experiments, and (6) to predict seepage into ventilated waste emplacement drifts.

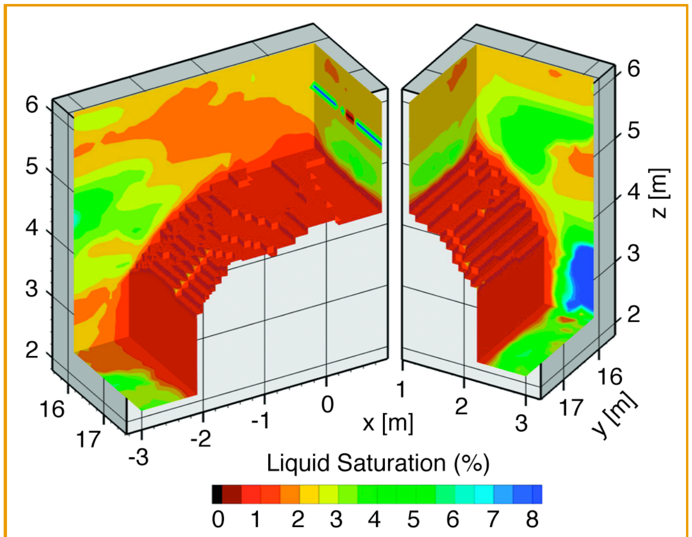

Figure 1. Saturation distribution around a ventilated underground opening, showing the dryout zone caused by evaporation effects

APPROACH

The research objectives are achieved by (1) monitoring relative humidity and ventilation conditions, (2) measuring evaporation potential, (3) observing wetting patterns at the drift ceiling during liquid-release tests, (4) implementing an evaporation boundary condition into an unsaturated flow simulator, (5) calibrating the model against evaporation and seepage data, and (6) using the calibrated model to estimate total evaporation rates and relating them to other terms affecting seepage.

ACCOMPLISHMENTS

We incorporated evaporation effects into the numerical simulator by modeling them as a saturation-dependent Fickian diffusion process. The evaporation boundary-layer thickness was then estimated based on data from free-water evaporation experiments conducted under known relative humidity, temperature, and ventilation conditions. A three-dimensional, heterogeneous fracture continuum model was developed to simulate liquid-release tests. The figure shows the saturation distribution under natural percolation conditions. Despite continuous downward flow of water, a dryout zone develops around the cavity (caused by the reduced relative humidity in the opening), preventing seepage from occurring and affecting the onset of dripping once water is injected from the borehole. The transient release of water from the borehole was simulated along with time-dependent changes in relative humidity. Seepage-relevant parameters were estimated by calibrating the model against the cumulative seepage amount observed in the opening. The modeling results indicate that evaporation effects in a ventilated tunnel are significant, i.e., they have to be accounted for during model calibration and predictive calculations.

SIGNIFICANCE OF FINDINGS

Compared to previous models that neglected the effect of evaporation, this new approach shows significant improvement in capturing observed seepage fluctuations into ventilated underground openings. Accounting for evaporation effects reduces the potential bias in the estimation of seepage-relevant parameters. It also allows for a better understanding of the mass balance during liquid-release tests, and thus provides more confidence in the use of the calibrated model for simulations of seepage under different ventilation conditions.

RELATED PUBLICATION

Ghezzehei, T., S. Finsterle, and R. Trautz, Evaluating the effectiveness of liquid diversion around an underground opening when evaporation is non-negligible. Proceedings of the TOUGH Symposium 2003, Berkeley, California, May 12–14, 2003.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and the Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab). The support is provided to Berkeley Lab through U.S. Department of Energy Contract No. DE-AC03-76SF00098.

Effects of Induced Convection on Far-Field Groundwater Flow

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RESEARCH OBJECTIVES

In the safety assessment of nuclear waste disposal, the influence of heat convection on the groundwater flow field cannot be neglected. This influence should be estimated by conducting a thermal-hydrological (TH) numerical analysis at the site characterization stage. However, as a first step, it is worthwhile to estimate the influence of heat convection using only the thermodynamic parameters obtained from existing data.

The objective of this research is to estimate the influence of heat convection on the natural groundwater flow system, employing a dimensionless parameter from case studies using a TH coupled model.

APPROACH

For this sensitivity study, the coupled heat and hydraulic simulation code TOUGH2 is applied to a vertical two-dimensional model with an area 10,000 m long and 3,000 m deep. Induced convection is generated by the hydraulic gradient (0.01) dictated by the assigned topography. The model is saturated with water, with a constant pressure at the upper boundary and impermeable lower and side boundaries. The upper and lower boundaries are set at a constant temperature, while side boundaries are insulated.

In this study, we use representative physical properties of a sedimentary rock. The vertical temperature gradient is set at 0.02°C/m. Variable permeabilities within two orders of magnitude are assigned to the model. From the results of case studies, we extract the average velocity along the particle stream traces from six starting points and the maximum vertical velocity in the model, and use them as qualitative indicators to evaluate the relative influence of heat convection. For comparison, we carried out simulations with the same hydraulic properties and the initial temperature distribution without heat transfer as the uncoupled model for each respective case.

ACCOMPLISHMENTS

To estimate the influence of thermal convection, we used the Peclet number, which denotes the ratio between advection and thermal diffusion. Figure 1 shows representative results from three cases depicting temperature distributions and stream traces. From these results, we can see that when the permeability is large, the recharge zone becomes larger, and the low-temperature area also becomes larger because of the increasing recharge of low-temperature water. Both the average velocity along the stream traces and the maximum vertical velocity increase as the Peclet number increases. However, the velocity ratios of the TH coupled model to the uncoupled model both decrease when the Peclet number exceeds 2.0.

In a high-permeability condition, the flow of cold water from the surface dominates the temperature distribution, and almost the entire area becomes a low-temperature zone. On the other hand, if the Peclet number is less than 0.2, the velocity ratio is less than 1.1, which means that the error in the uncoupled model is only about 10%.

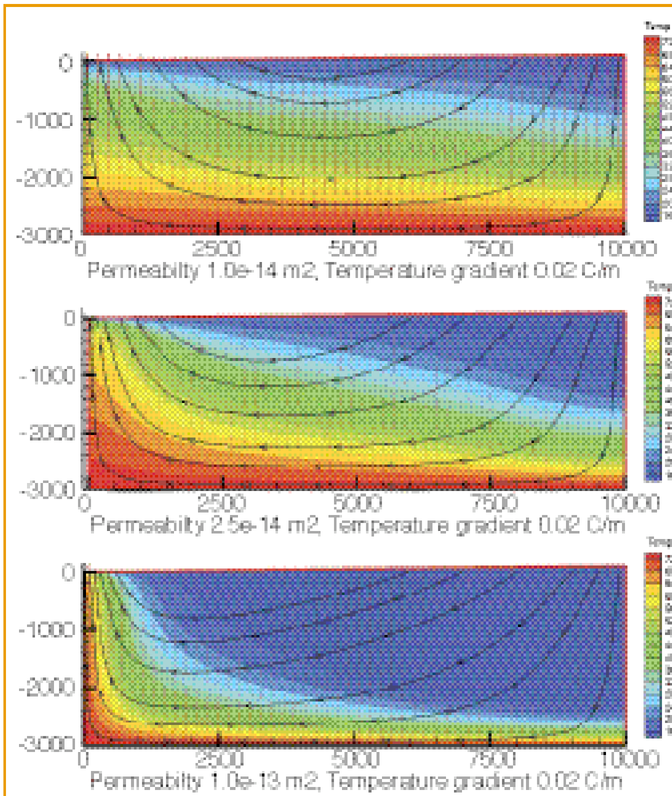

Figure 1. The temperature distribution and stream traces from three representative cases of coupled TH simulations with induced convection

SIGNIFICANCE OF FINDINGS

It was shown that the Peclet number is a useful indicator for predicting the influence of thermal convection on groundwater flow. When the Peclet number is small, the influence of heat convection is small because of the slow velocity. There is a critical Peclet number (a function of the topography) above which the influence of heat convection becomes significant.

ACKNOWLEDGMENTS

This work has been supported by Taisei Corporation under U.S. Department of Energy Contract No. DE-AC03-76SF00098.

Investigation of Uncertainty in Hydrogeologic Modeling of Flow and Transport in a Large, Saturated Granitic Rock Mass

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RESEARCH OBJECTIVES

The objectives of this project are: (1) to evaluate the uncertainty involved in modeling flow and transport in a large granitic rock mass, and (2) to seek ways of reducing that uncertainty.

APPROACH

A number of international research organizations are participating in this project. Each has been building a model and conducting simulations of groundwater flow and transport using the same set of information from a site in the Tono area of Gifu, Japan. The base data set is an accumulation of the past several years' field investigations and include geological, hydrological, geophysical, and geochemical data. As a new set of data becomes available, predicted flow rates and particle travel times through the model are compared among the different models. So far, flow rates and travel times differ by three to four orders of magnitude. One focus of the study is to find the cause of these differences among the models. Another focus is to evaluate how much the model improves as new data become available.

In our conceptual model, we use stochastic permeability and porosity distributions to represent fractured rock as an effective continuum. Only large-scale features such as fault zones, lithologic layering, natural boundaries, and surface topography are incorporated deterministically. Because the effective porosity of a large rock mass cannot be measured directly, it has to be estimated indirectly from several different types of data, using scientific judgment. Another large uncertainty stems from the hydraulic properties of faults, although some inferences can be made from measured hydraulic heads.

ACCOMPLISHMENTS

We have built and continuously updated a model that generally satisfies the observed pressure-head data. We have made use of temperature measurements to distinguish between two plausible boundary conditions for the model. The most recent update to the model was made using large-scale dynamic-pressure-disturbance data, which prompted us to increase the effective porosity value by fifty fold. We also expanded the boundary of our 4 km × 6 km × 3 km model to build a 9 km × 9 km × 2 km model. The latter appears to better define a hydrological basin. We used an inversion program, iTOUGH2, to estimate the permeability of a major fault by matching the steady-state head distribution.

SIGNIFICANCE OF FINDINGS

Our findings indicate that the hydraulic structure of the fault likely resembles a sandwich, with a low-permeability core and high-permeability zones on both sides of the core. This structure may generally describe reverse faults in a crystalline rock. Also, borehole temperature data may be used to reduce the uncertainties of a hydrological model. Finally, large-scale pressure disturbance data may be used to infer the effective permeability and porosity of a large fractured rock mass.

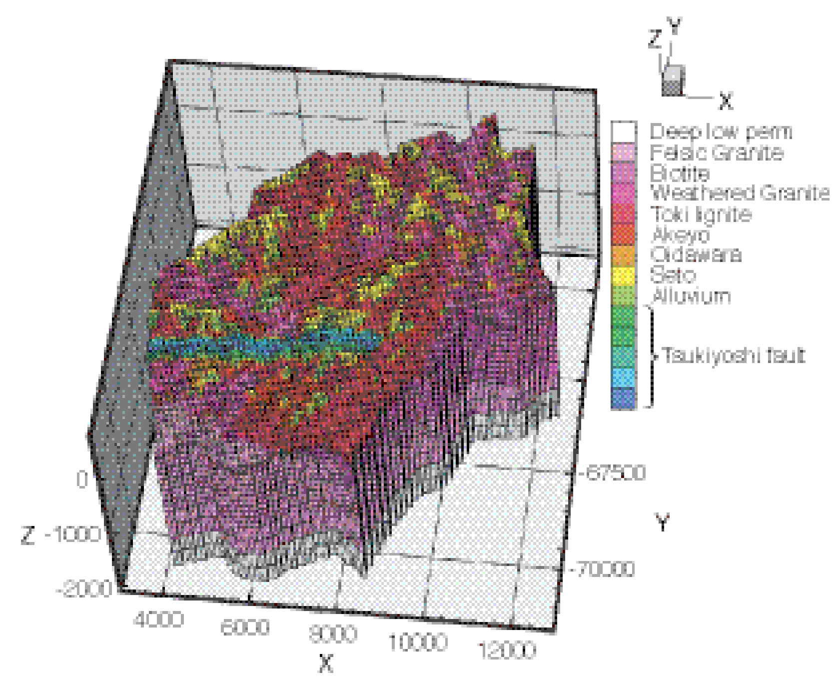

Figure 1. Three-dimensional perspective view of the model used for the TOUGH2 and iTOUGH2 simulations of the 9 km × 9 km × 2 km region. Material types are color-coded.

RELATED PUBLICATION

Doughty, C., and K. Karasaki, Constraining hydrologic models using thermal analysis. In: Proceedings, Rock Mech. Symp., Japan Society of Civil Engineers, Tokyo, Japan, January 23–24, 2003.

ACKNOWLEDGMENTS

This work was supported by the Japan Nuclear Fuel Cycle Corporation (JNC) and Taisei Corporation of Japan, through the U.S. Department of Energy Contract No. DE-AC03-76SF00098.

Fracture Sealing by Mineral Dissolution and Precipitation at Yucca Mountain

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RESEARCH OBJECTIVES

The emplacement of heat-generating waste at the proposed Yucca Mountain repository site will induce several processes to occur. Water naturally present in the rock will evaporate or boil, and this vapor will condense at a distance from the proposed repository, where the rock is cooler. The condensate will dissolve the host rock (tuff), and the dissolved constituents will precipitate if the water is boiled away. Mineral precipitation in fractures above the proposed repository could plug flow paths and reduce the probability of water seeping into the repository. Our research objectives are to provide a better understanding of (1) tuff dissolution under conditions expected in the proposed repository, (2) mineral precipitation in fractures, and (3) how these processes might affect the performance of such a proposed repository.

APPROACH

Our approach was to experimentally and numerically investigate tuff dissolution caused by water condensation in fractures and mineral precipitation in fractures subjected to a thermal gradient with a boiling region. We used anticipated temperature and pressure conditions in the proposed repository.

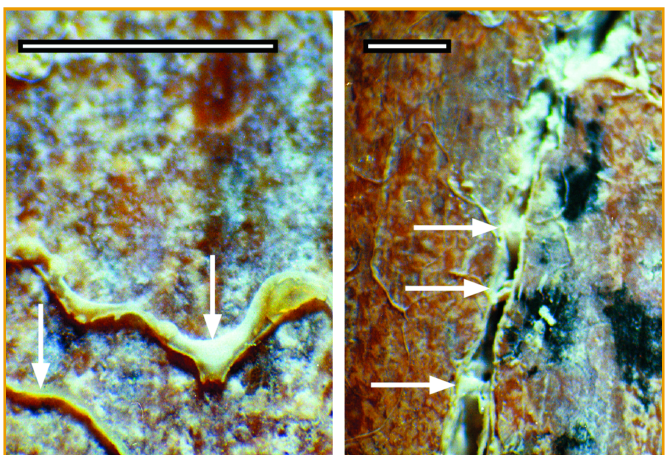

Figure 1. Bridging structures (identified with arrows): (a) extending outward from flat fracture face; (b) spanning aperture in cross-cutting natural fracture. Scale bars are 0.5 mm.

ACCOMPLISHMENTS

We replicated mineral dissolution by vapor condensate in fractured tuff by flowing water through crushed Yucca Mountain tuff at 94°C. We monitored the chemistry of the water passing through the crushed tuff to provide information on tuff dissolution. The steady-state fluid composition had a total-dissolved-solids content of about 140 mg/L, and silica was the dominant dissolved constituent. We flowed a portion of this mineral-laden water into a vertically oriented planar (saw cut) fracture in a block of welded Topopah Spring Tuff that was maintained at 80°C at the top and 130°C at the bottom. In the boiling region, the precipitation of amorphous silica from the water began to seal the fracture within 5 days. Upon opening the fracture, we observed the structure of the precipitate: precipitate coated the fracture walls and formed bridging structures that plugged the aperture. On the right side of Figure 1, we see bridging structures extending out from the fracture wall, and in the cross-cutting fracture shown on the left, both the fracture coating and bridging structures are visible.

A one-dimensional plug-flow numerical model was used to simulate mineral dissolution, and a similar model was developed to simulate the flow of mineralized water through a planar fracture, where boiling conditions led to mineral precipitation. Predicted concentrations of the major dissolved constituents for the tuff dissolution were within a factor of 2 of the measured average steady-state compositions. The mineral precipitation simulations predicted the precipitation of amorphous silica at the base of the boiling front, leading to a greater than 50-fold decrease in fracture permeability in 5 days, consistent with the laboratory experiment. These results help validate the use of a numerical model to simulate thermal-hydrological-chemical processes at Yucca Mountain.

SIGNIFICANCE OF FINDINGS

The experiment and simulations indicated that precipitation of amorphous silica could cause significant reductions in fracture porosity and permeability on a local scale. However, differences in fluid flow rates and thermal gradients between the experimental setup and anticipated conditions at Yucca Mountain need to be factored into scaling of the results.

RELATED PUBLICATION

Dobson, P.F., T.J. Kneafsey, E.L. Sonnenthal, N. Spycher, and J.A. Apps, Experimental and numerical simulation of dissolution and precipitation: Implications for fracture sealing at Yucca Mountain, Nevada. Journal of Contaminant Hydrology, 62–63, 459–476, 2003.

ACKNOWLEDGMENTS

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Scale Dependency of the Effective Matrix Diffusion Coefficient

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RESEARCH OBJECTIVES

The exchange of solute mass (through molecular diffusion) between fluid in fractures and fluid in rock matrix is called matrix diffusion. Owing to the order-of-magnitude slower flow velocity in the matrix compared to fractures, matrix diffusion can significantly retard contaminant transport in fractured rock. The effective matrix diffusion coefficient is an important parameter for describing this matrix diffusion, in that it largely determines overall contaminant transport behavior in fractured rock (in many cases). Such diffusion coefficient values measured from small-scale rock samples in the laboratory have been directly used for modeling large-scale radionuclide transport at the proposed Yucca Mountain nuclear waste repository site (and many other sites). However, some preliminary studies have indicated that field-scale matrix diffusion coefficient values are different from local values. The major objective of this work is to determine if a relationship exists between the effective matrix diffusion coefficient and test scales.

APPROACH

A number of field-scale tracer tests in fractured rocks have been conducted and interpreted by different research groups worldwide. Effective matrix diffusion coefficients, published in the literature and estimated from the relevant tracer tests, were surveyed. To detect the potential scale-dependence of the effective matrix diffusion coefficient, we compiled the ratio of an estimated effective matrix diffusion coefficient to its local value (corresponding to a small core sample) as a function of test scale (Figure 1).

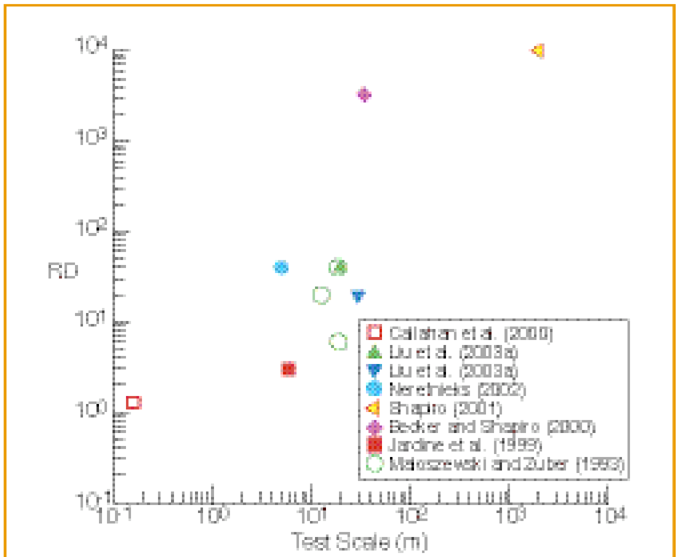

Figure 1. Effective matrix diffusion coefficient as a function of test scale. *RD* refers to the effective coefficient value (estimated from field data) divided by the corresponding local value.

ACCOMPLISHMENTS

As demonstrated in Figure 1, the effective matrix diffusion coefficient may be scale-dependent and generally increases with test scale. The mechanisms behind this surprising scale-dependency behavior are not totally clear. We offered a preliminary explanation based on the hypothesis that solute travel paths within a fracture network are fractals (Liu et al., 2003). We believe that the scale dependency of the effective matrix diffusion coefficient actually results from the scale dependency of the fracture-matrix interface area (as a result of fractal solute-travel paths).

SIGNIFICANCE OF FINDINGS

While the scale dependency of permeability and dispersivity has been known for many years in the subsurface hydrology community, we demonstrate—for the first time—that the effective matrix diffusion coefficient may also be scale-dependent, specifically increasing with test scale. This finding has many important implications for problems involving matrix diffusion. For example, the simulated radionuclide travel time within the unsaturated zone of Yucca Mountain may be significantly underestimated when this scale-dependent behavior is not considered. However, more carefully designed field tests and numerical experiments are still needed to confirm this scale-dependent behavior and to develop more rigorous theoretical explanations.

RELATED PUBLICATION

Liu, H.H., G.S. Bodvarsson, and G. Zhang, Scale dependency of the effective matrix diffusion coefficient. Vadose Zone Journal, 2003 (in press); Berkeley Lab Report LBNL-52824, 2003.

ACKNOWLEDGMENTS

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The Active Fracture Model and Fractal Flow Behavior

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RESEARCH OBJECTIVES

Continuum approaches are commonly used for modeling flow and transport in unsaturated fractured rocks. A traditional continuum approach assumes uniformly distributed flow patterns at a subgrid scale and therefore cannot be used for representing gravity-driven fingering flow and transport in fracture networks. In an effort to incorporate this figuring flow behavior into the continuum approach, Liu et al. (1998) developed the active fracture model (AFM), which assumes that only a portion of fractures in a connected unsaturated fracture network contributes to liquid water flow. The major objective of this work is to provide a further evaluation of the AFM, based on both theoretical arguments and field observations (Liu et al., 2003).

APPROACH

A flow system exhibits so-called fractal flow behavior when the corresponding flow patterns can be characterized by fractals. Many laboratory and field experiments have shown that complex fingering flow patterns in unsaturated porous media are fractal patterns. We used a box-counting approach to detect fractal flow patterns from spatial distributions within coated fractures (a sign of water flow within fractures) in the Yucca Mountain unsaturated zone (Figure 1). The theoretical relationship between the AFM and fractal flow patterns was also explored. AFM-based simulation results were then compared to C-14 and fracture coating data to check the validity of the AFM.

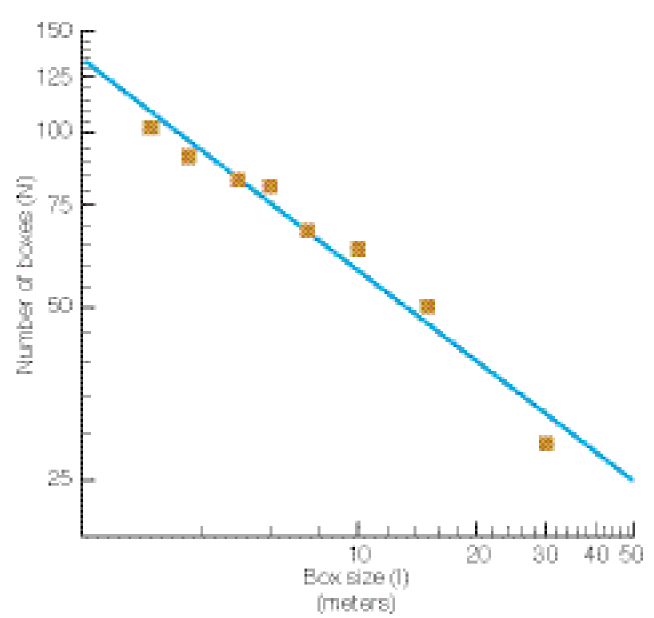

Figure 1. Relation between the number of boxes (N) covering at least one coated fracture, and box size l. The fitting of the solid line (corresponding to a power function) with the data points indicates a fractal pattern.

ACCOMPLISHMENTS

We demonstrated that flow patterns in unsaturated fractured rock, like those in unsaturated porous media, are fractal (Figure 1). While the AFM was initially developed as an empirical model, a rigorous theoretical relation between AFM and the fractal flow pattern was established. Comparisons between model simulations and the relevant field observations support the validity of the AFM.

SIGNIFICANCE OF FINDINGS

The inadequacy of numerical models in predicting fast flow and transport processes has been a significant problem for many unsaturated systems. In this work, we showed that complex unsaturated flow patterns in both porous media and fractured rock are fractal patterns, and that the AFM can capture this important behavior at the subgrid scale. Because of the relative simplicity of fractal-based characterizations, we believe that the fast flow behavior in unsaturated systems can be successfully captured by the improved large-scale continuum approach. This is partially supported by the consistency between simulation results based on the AFM and field observations from the Yucca Mountain unsaturated zone. Future work will focus on the possibility of extending the AFM to unsaturated porous media.

RELATED PUBLICATIONS

Liu, H. H., C. Doughty, and G. S. Bodvarsson, An active fracture model for unsaturated flow and transport in fractured rocks. Water Resour. Res., 34, 2633–2646, 1998.

Liu, H.H., G. Zhang, and G.S. Bodvarsson, The active fracture model: Its relation to fractal flow behavior and a further evaluation using field observations. Vadose Zone Journal, 2, 259–269, 2003.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and the Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab). The support is provided to Berkeley Lab through the U.S. Department of Energy Contract No. DE-AC03-76SF00098.

IMPLICATIONS OF HALIDE LEACHING ON CHLORINE-36 STUDIES AT YUCCA MOUNTAIN

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RESEARCH OBJECTIVES

Chlorine-36 generated from worldwide nuclear tests in the 1950s and 1960s has been used to identify fast flow paths at Yucca Mountain, Nevada, the proposed site for a national high-level nuclear waste repository. *Fast flow* refers to preferential transport of water through faults or fractures in surrounding rock media with relatively low permeability. Bomb-pulse ^{36}Cl carried into the subsurface by infiltrating rainwater presumably resides along fracture surfaces. However, leaching a rock sample to extract this salt inevitably extracts pore-water chloride (Cl) and rock chloride from the matrix as well. The work described here contributes to the understanding of leaching processes for the ongoing validation study of ^{36}Cl at Yucca Mountain.

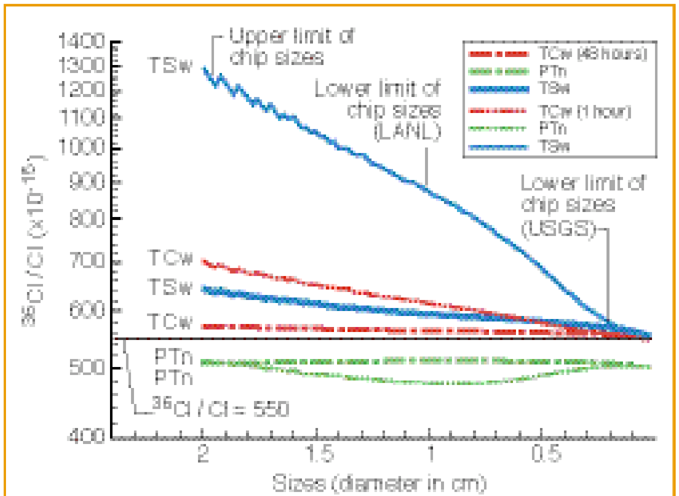

Figure 1. Model results indicating effects of chip size, leaching time, and rock pore water composition on ^{36}Cl/Cl for leachate at 1 hour and 48 hours simulated leaching time presented for rock samples from TCw, PTn, and TSw

APPROACH

In this work, we developed both a conceptual and numerical model (as well as a mathematical solution) for leaching processes. First, an analytical solution for diffusion of Cl and ^{36}Cl in composite media (rock matrix and water) was derived to accommodate variable diffusivity. Second, a leaching model was developed to take into account various Cl sources, including matrix pore water and less-easily-leached components (isolated fluid inclusion and mineral boundary salts). Third, the leaching model was applied to samples from Yucca Mountain stratigraphic units—the Tiva Canyon welded tuff (TCw), the Paintbrush nonwelded tuff (PTn), and the Topopah Spring welded tuff (TSw).

ACCOMPLISHMENTS

Our models successfully examined the role of sample leaching in the ^{36}Cl studies at Yucca Mountain. They simulated the effect of leaching time, sample size, and active and passive leaching. Model results show that the probability of detecting a ^{36}Cl/Cl bomb-pulse signal was severely diminished at longer leaching times and with smaller rock fragment sizes (Figure 1). Bomb-pulse signals in the TSw welded tuff were the least suppressed, because of lower concentrations in the pore water. However, bomb-pulse signals at TCw and PTn were "masked" (had limited detectability) because of higher matrix-pore-water Cl concentrations. Leaching times of 1 to 10 hours were more likely to reveal detectable bomb-pulse signals (if they were present). Bomb-pulse ^{36}Cl/Cl ratios were also more likely to be obtained when pore-water Cl concentrations were initially low.

SIGNIFICANCE OF FINDINGS

These research results demonstrate the effects of various factors in leaching experiments and provide much-needed theoretical guidelines for leaching protocols of ^{36}Cl study. The findings are expected to shed a great deal of light on the reproducibility debate in current ^{36}Cl validation studies.

RELATED PUBLICATIONS

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ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and the Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab). The support is provided to Berkeley Lab through the U.S. Department of Energy Contract No. DE-AC03-76SF00098.

3-D Studies of Mountain-Scale Radionuclide Transport in the Unsaturated Zone at Yucca Mountain, Nevada

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RESEARCH OBJECTIVES

The U.S. Department of Energy is actively investigating the technical feasibility of permanently disposing high-level nuclear waste in an appropriate repository proposed for the unsaturated zone (UZ) at Yucca Mountain, Nevada. The objectives of this study are to evaluate the transport of radioactive solutes and colloids under ambient conditions, from the proposed repository horizon to the water table, and to determine processes and geohydrological features that significantly affect radionuclide transport.

APPROACH

The radionuclide transport model considers the site hydrology and spatial distribution effects of hydraulic and transport properties in the Yucca Mountain subsurface. The migration and retardation of radionuclides are analyzed using EOS9nT (Moridis et al., 1999) and T2R3D (Wu et al., 1996), both of which are members of the TOUGH2 family of codes (Pruess, 1991). These models can describe the complex processes of flow and transport in the Yucca Mountain subsurface, including advection, diffusion, hydrodynamic dispersion, sorption, radioactive decay and tracking of daughters, colloid straining and physical-chemical filtration, and colloid-assisted solute transport. The mountain-scale grid for these 3-D studies of UZ transport consisted of 245,000 elements. A dual-permeability conceptualization was used to describe the fracture-matrix system in the UZ. The radioactive species were released directly into the fractures of the elements corresponding to the proposed repository. We investigated (a) instantaneous release, describing a single catastrophic event, and (b) continuous release, describing a plausible long-term scenario involving the breaching of the waste-containing canisters and the slow discharge of their contents. A total of eleven instantaneously released radionuclides were investigated, in addition to continuously released radioactive species that included four parents, two chains, and four colloids.

RESULTS

The results of the study indicate that the most important factors affecting radionuclide transport are the subsurface geology and site hydrology—i.e., the presence of faults (they dominate and control transport), fractures (the main migration pathways), and the relative distribution of zeolitic and vitric tuffs. Diffusion from the fractures into, and subsequent sorption onto, the matrix are the main retardation processes. Arrival times at the water table increase with the sorption distribution coefficients of the various species. For certain radionuclides such as ^{239}Pu, the contributions of the decay daughters to the total arrivals at the water table can be very significant. Changes in future climatic conditions can have a significant effect on transport, since increasing infiltration leads to faster transport to the water table. The transport of colloids is strongly influenced by their size (as it affects diffusion into the matrix, straining at hydrogeologic unit interfaces, and transport velocity).

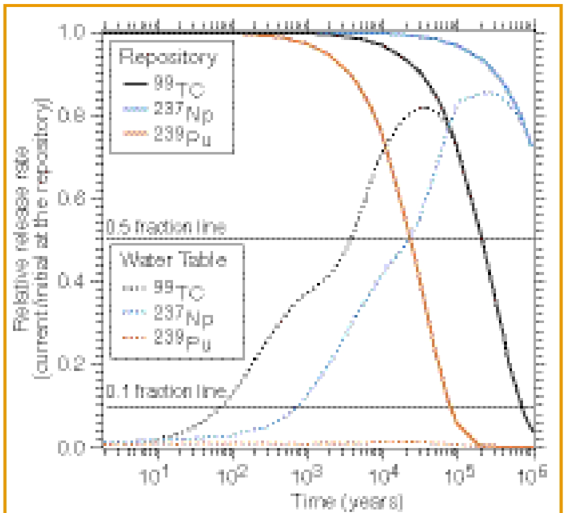

Figure 1. Normalized release rate of ^{99}Tc, ^{237}Np and ^{239}Pu from the repository horizon (for continuous release and mean present-day infiltration) and their subsequent arrival times at the water table

SIGNIFICANCE OF FINDINGS

Based on these studies, cumulative breakthrough curves for the radionuclides of interest were obtained. Note that because of the extremely conservative approach involved in this study, these curves describe the lower bound of arrival times at the water table.

RELATED PUBLICATIONS

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A Modeling Study of Flow Diversion and Focusing in Unsaturated Fractured Rocks

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RESEARCH OBJECTIVES

In a complex subsurface system with multiple layers, faults, and spatially varied alteration of rock properties, flow diversion and focusing are natural phenomena. However, quantitatively describing the magnitude and the spatial patterns of flow diversion and focusing is a challenge for both measurements and modeling. The objective of this study is to develop a systematic modeling approach, taking the Yucca Mountain unsaturated zone (UZ) as an example, to analyze and describe flow diversion and focusing in unsaturated fractured rocks, under ambient steady-state flow conditions.

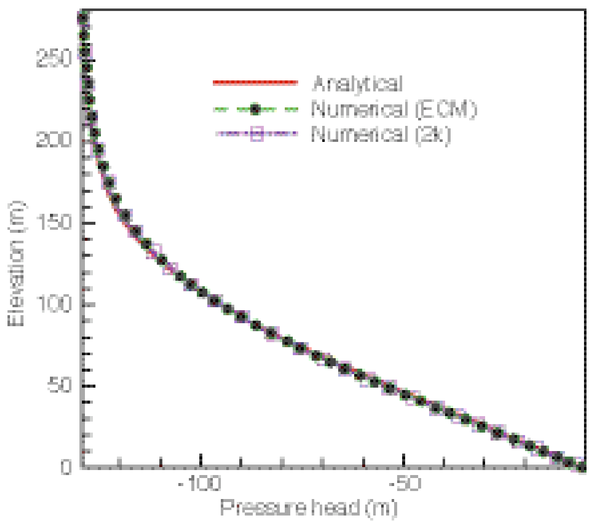

Figure 1. Comparison of pressure-head profiles in the PTn23 layer, calculated using analytical and numerical solutions

APPROACH

We first approximated the fractured tuffs of Yucca Mountain using the effective continuum model (ECM). For this, we used analytical solutions to identify the critical layers and layer interfaces in terms of flow diversion and to estimate the potential magnitudes of such diversion at typical locations. Then, we approximated the fractured tuffs as dual-permeability media and developed a large 3-D numerical grid (over one million gridblocks) to incorporate the site-specific data (including the knowledge obtained from the analytical solutions). The parallel-computing version of TOUGH2 was used to perform the numerical modeling, and the 3-D numerical modeling results were partly verified with field measurements.

ACCOMPLISHMENTS

We extended the analytical solutions of capillary barriers derived by Warrick et al. (1997) for porous media to the case of fractured media (under the ECM approximation) represented by specific geological units (and layers within those units) at Yucca Mountain. The analytical solutions show that, under present-day ambient conditions, capillary diversion occurs primarily within nonwelded units (i.e., units where matrix flow is dominant), like the Paintbrush nonwelded tuff (PTn) unit at Yucca Mountain. Among the critical rock layers within that unit, PTn21, PTn23, and vitric Calico Hills-1 (CH1) conduct the most down-dip diversionary flow, whereas PTn22, PTn24, and vitric CH2 act as capillary barriers to the downward percolation flux. Under dry, ambient conditions, the analytical solutions are good approximations of the capillary barrier system of fractured tuffs (Figure 1).

The 3-D numerical flow model developed in this study is (up to now) the most detailed site-scale model of the Yucca Mountain UZ over several decades of site study. The numerical simulations show that, although the net infiltration rate at the surface depends on various factors, including topography, soil thickness, vegetation, and rock type, the percolation flow patterns are considerably modified during transit through the thick unsaturated zone and are primarily controlled by a few critical rock layers and faults.

SIGNIFICANCE OF FINDINGS

The results show that:

1. The analysis that combines analytical solutions with large-scale numerical modeling is effective for analyzing and describing flow diversion and focusing in unsaturated rock.
2. Large-scale lateral flow could take place in the UZ at Yucca Mountain under ambient conditions. The combined effects of horizontal and vertical barriers result in generally reduced percolation flow through the proposed repository horizon, but also in flow focused downward along penetrating faults.
3. Because lateral flow occurs within a few layers and often turns into focused vertical flow via faults in the models, more detailed information about them is critical to fully understand and describe flow diversion and focusing in the UZ.

RELATED PUBLICATION

Pan, L., Y.-S. Wu, and K. Zhang, A modeling study of flow diversion and focusing in unsaturated fractured rocks. Vadose Zone Journal, 2002 (submitted); Berkeley Lab Report LBNL-49274, 2002.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and the Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab). The support is provided to Berkeley Lab through the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

New Improvements to WinGridder: An Interactive Grid Generator For TOUGH2

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RESEARCH OBJECTIVES

The objective of this study is to enhance the WinGridder software program, which acts as a grid generator for TOUGH2, a software program used worldwide as a simulation code for multiphase, multicomponent flow and heat transfer. The main objectives are (1) to add the capability of handling a repository with multiple subregions and specified drifts, (2) to incorporate an interpolation method (instead of picking the nearest point) in calculating the geological data from a given digital geological model, (3) to add the capability of generating multiple continuum grids (MINC grids), and (4) to enhance searching and other capabilities.

APPROACH

The following approaches were adopted:

1. Taking advantage of the object-oriented-programming used in WinGridder coding, we modified the REPOSITO object to include subobjects, labeled REGIONS and DRIFTS, to represent subregions and emplacement drifts. In this way, WinGridder could handle a repository with multiple subregions, with each region having specified drifts. As a byproduct, additional grid cells representing any user-specified drifts could be embedded into an existing 3-D grid.
2. A modified bilinear interpolation method (allowing for special treatment in the neighborhood of a fault) has been implemented in the member function of the LAYER object, which calculates the geological data (e.g., layer thickness or elevation).
3. The MINC grid generated by WinGridder is similar in principle to that of the dual-continuum grid. The difference is that the matrix cell in a dual-continuum grid is split into N (a number specified by the user) connected subcells in the corresponding MINC grid. The fracture configurations (e.g., fracture porosity, fracture-matrix interface area per rock volume, fracture aperture and spacing) are provided by the user in a text file. (This functionality is only available in WinGridder V2.1 (beta)).
4. The Save Submesh functionality has been enhanced to save any user-selected subgrid as an independent grid project. Many other tools have been added.

ACCOMPLISHMENTS

WinGridder V2.0 and V2.1 (beta) have been developed, and WinGridder V2.0 has been qualified for the Yucca Mountain Project. V2.0 has been successfully used to design and generate 1-D, 2-D, and 3-D meshes for numerical modeling of flow and transport at Yucca Mountain and at the Berkeley Lab site.

SIGNIFICANCE OF FINDINGS

The main advantages of this grid-generation software are its user-friendly graphical interfaces, flexible grid-design capabilities, efficient grid generation, and powerful searching and postprocessing capability, especially for large size grids (e.g., grids composed of a million grid cells or more). This software has been increasingly applied around the world (so far, multiple users in the U.S., Asia, and Europe).

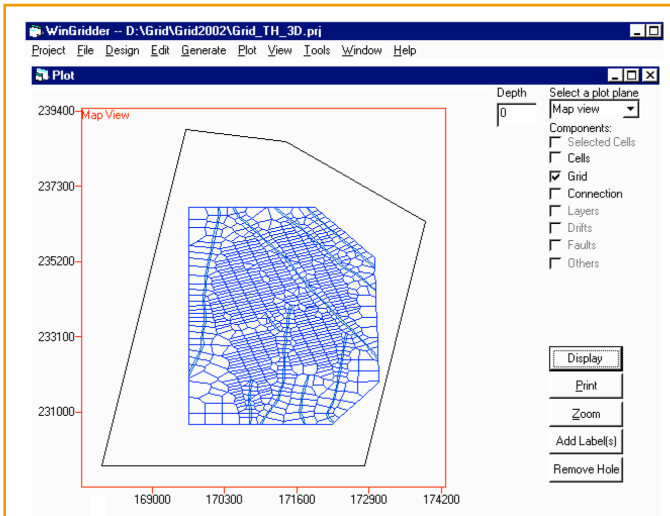

Figure 1. The main window of the WinGridder.

RELATED PUBLICATION

Pan, L., WinGridder—An interactive Grid Generator for TOUGH2. Proceedings of the TOUGH Symposium 2003. Berkeley, California, May 12–14, 2003; Berkeley Lab Report, LBNL-52422, 2003.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and the Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab). The support is provided to Berkeley Lab through the U.S. Department of Energy Contract No. DE-AC03-76SF00098.

Coupled Thermal-Hydrological-Mechanical Analysis with TOUGH-FLAC

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RESEARCH OBJECTIVES

The objective of this work is to develop a numerical simulator for coupled thermal-hydrological-mechanical (THM) analysis of complex geological media under multiphase flow conditions, with possible coupling to reactive transport modeling.

APPROACH

Two existing computer codes—TOUGH2 and FLAC-3D—were joined to develop a numerical simulator (named TOUGH-FLAC) for analysis of coupled THM processes in complex geological media under multiphase flow conditions. Both codes are well established and widely used in their respective fields. The TOUGH2 code is designed for geohydrological analysis of multiphase, multicomponent fluid flow and heat transport, whereas the FLAC-3D code is designed for rock and soil mechanics with thermomechanical and hydromechanical interactions. The two codes are executed on two separate meshes and joined with two coupling modules (Figure 1). A set of coupling modules can be exchanged with another set, depending on the type of rock and the studied problem.

ACCOMPLISHMENTS

A set of TOUGH-FLAC coupling modules has been developed for various applications. Recent applications of the TOUGH-FLAC simulator include:

- A study of caprock hydromechanical changes associated with CO_2 injection into a brine formation
- A study of the impact of coupled THM processes on the performance of the proposed nuclear waste repository at Yucca Mountain, Nevada, including drift-scale and mountain-scale coupled THM processes
- Coupled THM analysis of the Yucca Mountain Drift Scale Test
- Analysis of surface uplift during volcanic episodes
- A study of fault slip during underground injection CO_2 (ongoing)

SIGNIFICANCE OF FINDINGS

A coupled THM numerical simulator for multiphase flow conditions has been successfully constructed and its use demonstrated. The results from these simulations will be important for the performance assessments of geological disposal of CO_2 and spent nuclear fuel, and are also valuable in other applications (such as geothermal energy extraction and oil and gas reservoir engineering).

RELATED PUBLICATIONS

Rutqvist, J., Y.-S. Wu, C.-F. Tsang, and G. Bodvarsson, A modeling approach for analysis of coupled multi-phase fluid flow, heat transfer, and deformation in fractured porous rock. Int. J. Rock Mech. Min. Sci., 39, 429–442, 2002.

Rutqvist, J., and C.-F. Tsang, A study of caprock hydromechanical changes associated with CO_2 injection into a brine aquifer. Environmental Geology, 42, 296–305, 2002.

Rutqvist, J., and C.-F. Tsang, Analysis of thermal-hydrological-mechanical behavior near an emplacement drift at Yucca Mountain. J. Contaminant Hydrology, 62–63,1–16, 2003.

ACKNOWLEDGMENTS

This work was jointly supported by the Director, Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences and Biological Sciences, of the U.S. Department of Energy, under Contract No. DE-AC03-76-SF00098; and by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and the Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab). The support is provided to Berkeley Lab through the U.S. Department of Energy Contract No. DE-AC03-76SF00098.

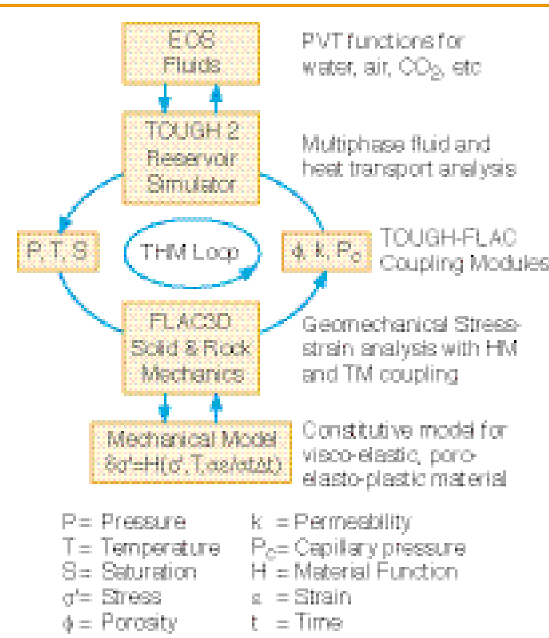

Figure 1. Schematic of linking TOUGH2 and FLAC3D for a coupled THM simulation

Flow and Transport Through a Fault Embedded in Fractured Rock

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RESEARCH OBJECTIVES

The overall objective of this investigation is to study flow and transport through a 20 m vertical section of a fault located in the fractured welded tuff of the Topopah Spring welded tuff unit at Yucca Mountain, Nevada (Figure 1), the proposed site for a high-level nuclear waste geologic repository.

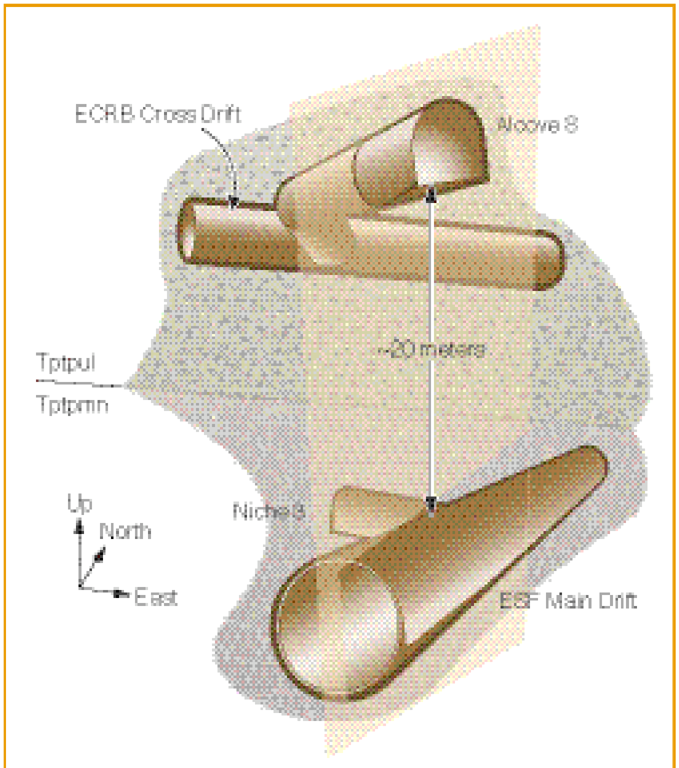

Figure 1. Location of the test bed between the Cross Drift and Main Drift in the Exploratory Studies facility. Shaded plane is located along presumed location of fault.

APPROACH

This investigation involved the release of approximately 82,000 liters of water along a horizontal section of the fault, under ponded conditions over a period of thirteen months and then under reduced fluxes for another six months. When quasi-steady-state seepage was observed at the lower end of the test bed, two tracers with different molecular diffusion coefficients were introduced into the ponded water infiltrating the fault. After tracer-laced water had been released into the fault, more tracer-free water was released. As water was released into the fault, changes in moisture content were monitored in the formation, while a large cavity excavated below the test bed was visually inspected for seepage. Water percolating through the fault and into the excavated cavity was continuously monitored with an automated, remotely accessed water collection system.

ACCOMPLISHMENTS

We observed that water (introduced along the fault) followed the fault as the primary vertical flow path, while the adjacent fractured matrix served to move water laterally and vertically. Unlike primary flow paths along the fault, flow was not persistent along the secondary flow paths under similar boundary conditions. The field experiment showed the existence of a capillary barrier and confirmed the dynamic nature of flow through the fault. Further, observations of bromide concentrations in seepage water during the early stages of the experiment, and of bromide and pentafluoride benzoic acid (PFBA) concentrations in the seepage water, indicate the significant influence of matrix diffusion on transport through a fault embedded in fractured, nonwelded rock.

SIGNIFICANCE OF FINDINGS

Field tests involving both flow and transport within a fault under unsaturated conditions are rare. This test has provided insights into mechanisms that come into play when water with tracers is introduced into a fault located in this unsaturated environment. This information is being used to develop conceptual models of flow and transport through Yucca Mountain.

RELATED PUBLICATIONS

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Salve, R., A passive-discrete water sampler for monitoring seepage. Groundwater, 2003 (in press); Berkeley Lab Report LBNL-51203, 2002.

ACKNOWLEDGMENTS

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A Numerical Study of Unsaturated Flow and Transport Through a Fractured Meter-sized Rock Block

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RESEARCH OBJECTIVES

Our work involves study of a meter-sized block of fractured rock to obtain experimental evidence in support of the active fracture concept (AFC). This concept assumes that only a portion of fractures in a connected unsaturated fracture network contributes to liquid water flow. Prior to this experimental evaluation, however, we needed to perform a preliminary numerical simulation in which we incorporated the AFC into a dual-continuum model (DCM) to create an enhanced DCM. Through this integration, we intend to identify the most effective way to quantify the AFC parameter in the laboratory.

APPROACH

The DCM was developed and then compared to a discrete fracture network model (DFNM) representing the meter-sized rock block, to see whether the DCM could accurately simulate flow and transport in the block. The DFNM, which contained an artificially generated 2-D fracture network, is based on statistical information from field observations at Yucca Mountain, Nevada (including fracture density, ranges of aperture and trace length, distribution of orientation, flow rate, and tracer transport data). As a preliminary step, DCM results obtained without incorporating the AFC were calibrated against the DFNM data. The AFC model was then integrated into the DCM to examine whether adding the AFC model could improve DCM predictions of discrete flow behavior.

ACCOMPLISHMENTS

At transient states, the DFNM showed distinctive preferential flow patterns, such as stepwise increases in water effluent flow rates and high water saturation along predominant flow paths (i.e., fractures). The DCM breakthrough curves did not initially capture the DFNM results because of their conceptual differences. But after the incorporation of the AFC, DCM predictions for flow-rate breakthrough curves were significantly improved. The flow rates from the AFC-enhanced DCM were calibrated against those of the DFNM to estimate the effect of including the AFC parameter.

SIGNIFICANCE OF FINDINGS

These numerical simulations imply that laboratory experiments incorporating a transient state in the flow field would provide a more sensitive approach for estimating the AFC parameter than steady-state experiments. Additionally, water breakthrough curves at low (rather than high) injection rates may be more appropriate for laboratory tests to determine the AFC parameter. The results also suggest that the DCM-AFC approach improves the prediction of unsaturated flow and transport, but may not be well suited for the current two-dimensional meter-scale model. Three-dimensional studies with detailed characterization of fracture networks have been proposed for more accurate estimation of the AFC parameter.

RELATED PUBLICATIONS

Seol, Y., T.J. Kneafsey, K. Ito, and S. Finsterle, Simulation of unsaturated flow and transport through a fractured meter-sized model block using the continuum approach. Water Resources Research, 2003 (submitted); Berkeley Lab Report LBNL-52818, 2003.

Ito, K., and Y. Seol, A 3-D discrete fracture network generator to examine fracture-matrix interaction using TOUGH2. Proceedings of the TOUGH Symposium 2003, Berkeley, California, May 12-14, 2003; Berkeley Lab Report LBNL-52465, 2003.

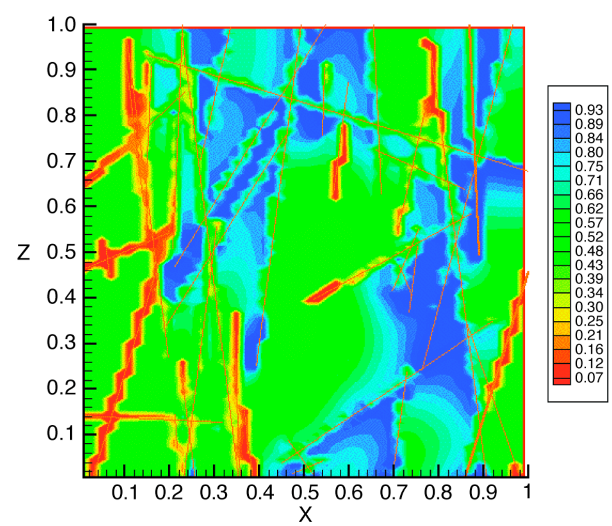

Figure 1. Distribution of water saturation in the DFNM, showing preferential flow patterns developed along major fractures in the transient state of the flow domain.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and Berkeley Lab. The support is provided to Berkeley Lab through the U.S. Department of Energy Contract No. DE-AC03-76SF00098.

Effects of Water-Rock Interaction of Unsaturated Flow in Heterogeneous Fractured Rock

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RESEARCH OBJECTIVES

Evaluation of coupled thermal, hydrological, and chemical processes associated with the proposed high-level nuclear waste repository at Yucca Mountain, Nevada, requires consideration of the effects of permeability heterogeneity on reaction-transport processes. The primary objective of this work is to examine the relationship of fracture flow and fracture-matrix interaction to permeability and capillary pressure modification during mineral precipitation and dissolution in unsaturated fractured tuff under boiling conditions.

APPROACH

In this analysis, we relate the reactive surface area to the fracture-matrix interaction area, based on a modified form of the Active Fracture Model for flow in unsaturated fractured rock. In most experimental and natural systems, permeability reductions to values near zero occur at porosities significantly greater than zero. This generally is the result of mineral precipitation preferentially closing the narrower interconnecting apertures. The hydraulic aperture, calculated from the fracture spacing and permeability (as determined through air-permeability measurements) assuming a cubic law relation, was used to develop a much stronger relationship between permeability and porosity. Based on air-permeability measurements, 2-D heterogeneous fracture permeability fields were generated having a range of four orders of magnitude. Reaction-transport simulations were performed using TOUGHREACT, which included coupling between heat, water, and vapor flow; aqueous and gaseous species transport; and kinetic and equilibrium mineral-water reactions. Changes in unsaturated flow take place through coupling of porosity, permeability, and capillary pressure to mineral precipitation/dissolution.

ACCOMPLISHMENTS

Simulations demonstrated that in addition to thermodynamic and geochemical parameters, the extent of mineral-water reaction is a function of the fluid flux and the liquid saturation. Liquid saturations, which control reactive surface areas, and fluxes are strongly tied to the permeability and capillary properties. At the edge of the boiling front, mineral precipitation is driven by a combination of mineral-water-reactions and evaporative concentration. The net effect of these processes over 20,000 years is a reduction in permeability that is most pronounced in areas of initially low permeability but high liquid fluxes and saturation (Figure 1). The distribution of permeability changes is, however, a combined effect of different minerals precipitating in varying patterns. Amorphous silica, calcite, and gypsum precipitate by evaporative concentration at the boiling front, resulting in a narrow zone of reduced permeability. Calcite also precipitates by degassing of CO_2 and heating of percolating fracture water from the surface, thus leading to abundant precipitation well above the boiling zone.

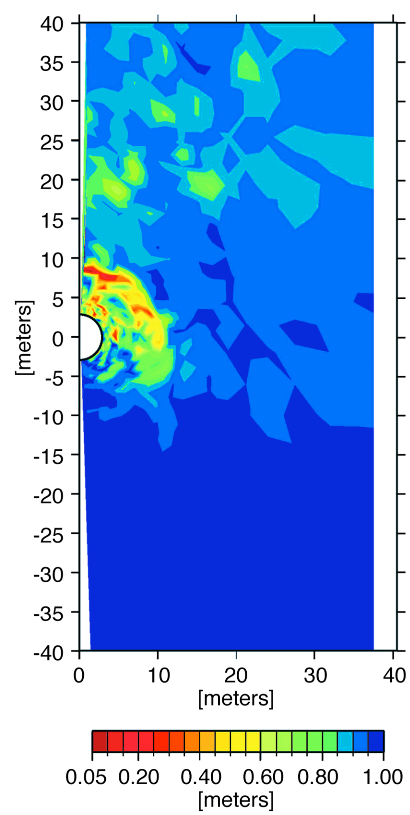

Figure 1. Ratio of fracture permeability at 20,000 years to the initial value

SIGNIFICANCE OF FINDINGS

Modeling of water-rock interaction in boiling, unsaturated, heterogeneous fractured rock exemplifies the strong feed-backs between water-rock interaction and unsaturated flow. In particular, increased liquid saturation, as a result of higher capillary pressures in smaller aperture fractures, leads to increased rates of reaction and further reductions in permeability. This work indicates that the evolution of preferential flow paths in unsaturated systems undergoing water-rock interaction may progress from the smaller features to the larger ones, in contrast to saturated systems that tend to start with the most permeable features.

RELATED PUBLICATION

Sonnenthal, E., N. Spycher, and T. Xu, Linking reaction, transport, and hydrological parameters in unsaturated fractured rock: TOUGHREACT implementation and application. Proceedings of the TOUGH Symposium, Berkeley, California, May 12-14, 2003.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and the Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab). The support is provided to Berkeley Lab through the U.S. Department of Energy Contract No. DE-AC03-76SF00098.

Yucca Mountain Heater Test Cooling Phase

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RESEARCH OBJECTIVES

As part of a multilaboratory team, Berkeley Lab is conducting a large-scale *in situ* thermal test, the Drift Scale Test (DST), in an underground facility at Yucca Mountain, Nevada, the site for a proposed national high-level nuclear waste repository. The test is presently in the second year of the natural cooling phase following four years of heating, during which an approximate heating rate of 185 kW was supplied by nine canister heaters (placed in a drift 47.5 m in length and 5 m in diameter) and fifty 11 meter long rod heaters installed in boreholes drilled perpendicular to the drift. The heating thus provided set in motion coupled thermal (T), hydrological (H), chemical (C), and mechanical (M) processes of the type that would be generated from heating in the proposed repository during its postclosure performance period. The objective of this test is to gain an in-depth understanding of THMC coupled processes within fractured welded volcanic tuff situated above the water table.

APPROACH

The DST has involved a close integration of measurements and numerical modeling. Thousands of sensors installed in nearly 100 boreholes, within a rock block of 60 × 60 × 60 m^3, continuously monitor the temperature, relative humidity, and mechanical displacement. Geophysical and air-permeability measurements have been performed at quarterly intervals to track moisture redistribution resulting from boiling, vapor transport, and condensation. Water and gas samples have also been collected periodically from the test block for chemical and isotopic analyses. In addition, TH, THC, and THM processes have been simulated using numerical models that realistically incorporate the three-dimensional test configuration and the complex multiple processes. Model predictions have been compared to the aforementioned extensive set of measured data.

ACCOMPLISHMENTS

Manifestations of coupled THMC processes in the rich set of measured data agree well with TH, THC, and THM model predictions. During the heating phase, expanding zones of reduced liquid saturation in the rock matrix around the heaters predicted by TH simulations were consistent with zones of drying shown in neutron logging data, crosshole radar tomograms, and electrical resistivity tomography data. During (the ongoing) cooling, the geophysical data has indicated slow rewetting at the edge of the drying zone, consistent with model predictions. Simulated fracture liquid-saturation has indicated that little water is likely to be collected during the cooling phase, as has been the case. Figure 1 shows the simulated and measured temperatures at the end of the heating phase and after six months of cooling in three boreholes. The plateau at the nominal boiling temperature of ~97°C indicates a liquid and vapor two-phase zone that is a good candidate for water collection. Note the disappearance of these two-phase zones during the cooling phase. Air-permeability measurements confirm modeled predictions of TH processes (drying and wetting in fractures) and THM processes (closing and opening of fractures).

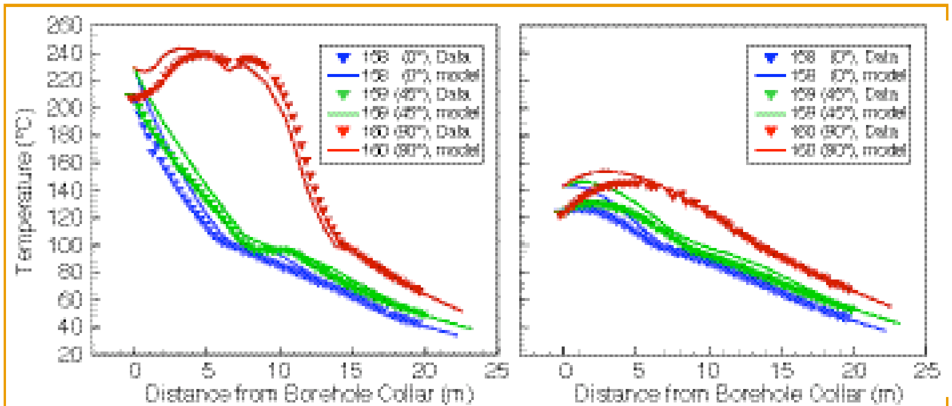

Figure 1. Simulated and measured temperature profiles in boreholes 158, 159, and 160, at (a) 48 months of heating and (b) 6 months of cooling

SIGNIFICANCE OF FINDINGS

A close integration of measurements and sophisticated simulations carried out in this large-scale and long-term test has contributed much toward the understanding of THMC coupled processes in fractured rock of the unsaturated zone.

RELATED PUBLICATION

Birkholzer, J.T., and Y.W. Tsang, Modeling the thermal-hydrological processes in a large-scale underground heater test in partially saturated fractured tuff. Water Resour. Res., 36(6), 1431–1448, 2000.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and the Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab). The support is provided to Berkeley Lab through U.S. Department of Energy Contract No. DE-AC03-76SF00098.

A Mountain-Scale Flow Model for the Unsaturated Zone of Yucca Mountain, Nevada

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RESEARCH OBJECTIVES

Large-scale 3-D flow models have played a critical role in characterizing and assessing the effects of hydrogeologic, thermal, and geochemical conditions in the unsaturated zone (UZ) at Yucca Mountain, Nevada, the proposed site of the future U.S. nuclear waste repository. Our work involves developing and refining the current mountain-scale UZ flow model developed for use in the current Total System Performance Assessment for License Application (TSPA-LA) in connection with Yucca Mountain.

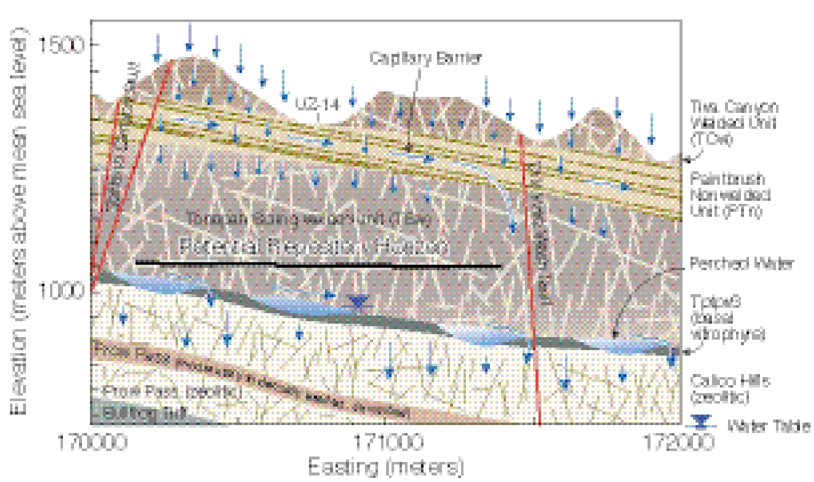

Figure 1. Schematic showing the conceptualized flow processes

APPROACH

The methodology employed in the ongoing development of the mountain-scale UZ flow model, based on the conceptual model (Figure 1), follows an iterative approach:

- Design a proper 3-D grid that incorporates complicated geological features of the site.
- Incorporate all available field data collected from the UZ.
- Calibrate the model using field-measured hydrological, pneumatic, thermal, and geochemical data.
- Conduct predictive studies and sensitivity analyses.

The modeling approach used in the UZ flow model is a dual-continuum mathematical formulation of coupled multiphase fluid and tracer transport through fractured porous rock, developed with the TOUGH2 code (a simulation code for multiphase, multicomponent flow and heat transfer).

ACCOMPLISHMENTS

Site-scale UZ flow models and submodels have shown the ability to match various types of field data on the model scale, including matrix liquid saturation and water potential, perched-water elevations, pneumatic data, geothermal gradients, and chloride data. The model has been used to (1) integrate all the available data from the UZ system into a single, comprehensive, and calibrated 3-D model for simulating the hydrological, thermal, and geochemical conditions at Yucca Mountain—for use in predicting system responses to ambient and future climate conditions; (2) quantify the moisture flow through the UZ, under present-day and estimated future climate scenarios; and (3) calculate times of radionuclide transport from the proposed repository level to the water table.

The site-scale UZ model has been successfully used to simulate past, present, and future hydrogeological, geothermal, and geochemical conditions and physical processes within the Yucca Mountain UZ. This model can be used to support various TSPA-LA activities.

SIGNIFICANCE OF FINDINGS

The mountain-scale UZ flow model generates 18 three-dimensional steady-state UZ flow fields, which have been used in direct calculations of radionuclide transport from the proposed repository to the water table, to support the TSPA-LA efforts. In addition, the UZ model results provide input parameters to various small-scale models and studies, such as drift-scale models, the mountain-scale thermal-hydrological model, and the UZ radionuclide transport model.

RELATED PUBLICATIONS

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Wu, Y. S., G. Lu, K. Zhang, G. Zhang, H.H. Liu, T. Xu, and E. L. Sonnenthal, UZ flow models and submodels. Report MDL-NBS-HS-000006 REV01, Lawrence Berkeley National Laboratory, CRWMS M&O, Berkeley, CA; Las Vegas, Nevada, 2003.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and the Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab). The support is provided to Berkeley Lab through the U.S. Department of Energy Contract No. DE-AC03-76SF00098.

A Numerical Investigation of Flow Focusing in Unsaturated Fracture Networks

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RESEARCH OBJECTIVES

The primary objective of this work is to develop numerical models to improve our understanding of discrete flow paths through unsaturated fracture networks. These fracture networks are modeled using fracture data collected from the Topopah Spring welded tuff unit (TSw) of Yucca Mountain, Nevada, the site of the proposed national nuclear waste repository. We try to answer the following questions: How do flow paths develop in the randomly distributed fracture network? How do rock matrix and infiltration rate (on the top boundary) influence flow patterns in the fracture networks? And finally, what is the relation between flow focusing and boundary conditions?

APPROACH

A two-dimensional fracture network was constructed using field fracture-mapping data, including fracture density, length range, and fracture orientations measured at the site. Each fracture in the network is randomly distributed; however, the random distribution is governed by statistical information derived from field-measured fracture data. Statistically, the generated fracture network should correspond to actual fracture distribution in the study domain. Figure 1 shows a fracture network consisting of those fractures intersecting globally connected paths. Isolated fractures are neglected in the simulation. The simulation domain is considered to be combined media, consisting of a fracture network superimposed on a porous matrix.

ACCOMPLISHMENTS

Five simulation cases were run with different matrix rock permeabilities and different infiltration rates. These cases may reflect the influence of matrix rock on flow focusing and the influence of infiltration rate on the flow pattern of the fracture network. The modeling results demonstrate that focused flow paths through fractures are generally vertical (Figure 1). Simulation results suggest that the average spacing between flow paths in a layered system tends to increase with depth as long as flow is gravity-driven. In addition, flow paths are found to consist primarily of long trace fractures in lower fracture-density domains. In higher fracture-density domains, long and short trace fractures both contribute to the development of flow paths.

SIGNIFICANCE OF FINDINGS

The majority of fluxes along flow paths have low normalized fluxes (ranging from 0 to 2). The higher normalized flux is caused by the higher degree of focusing into several fracture paths. Simulation results indicate that lower matrix-rock permeability will lead to a larger flow-focusing phenomenon. Flow focuses into only a few fractures and forms two main flow paths. Each flow path spreads over a range of several meters. Simulation results thus indicate that the impact of infiltration rate on flow focusing may be insignificant for unsaturated flow in a fracture network.

RELATED PUBLICATIONS

Zhang, K., Y.S. Wu, G.S. Bodvarsson, and H.H. Liu, Flow focusing in unsaturated fracture networks: A numerical investigation. Vadose Zone Hydrology, 2003 (in press); Berkeley Lab Report LBNL-52819, 2003.

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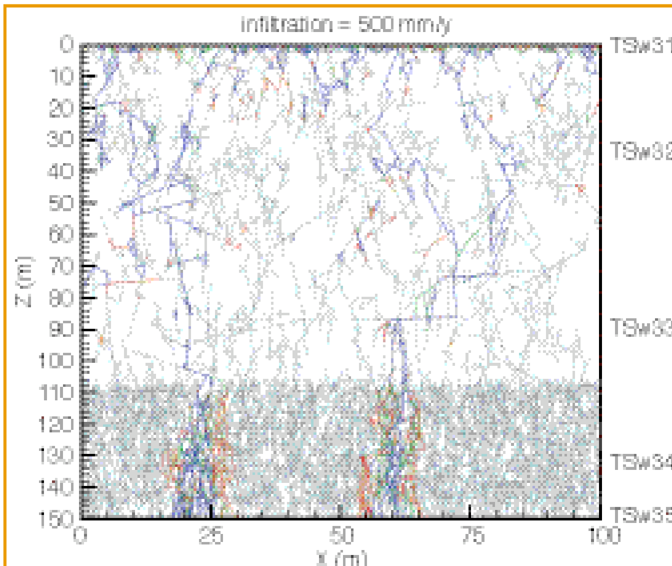

Figure 1. Simulated steady-state flux distribution in the fracture network, matrix permeability = 0; infiltration rate = 500 mm/year. Flux magnitude is represented by four different colors (in decreasing sequence): blue, green, red and grey. Each color represents a one-order-of-magnitude difference in flux.

ACKNOWLEDGMENTS

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Multiscale Heterogeneity Effects at Yucca Mountain

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RESEARCH OBJECTIVES

The objectives of this work are to characterize the multiscale variability of fracture and matrix hydrogeological properties, and to investigate the effects of multiscale heterogeneity on unsaturated flow and transport at Yucca Mountain, Nevada, the proposed site for the national high-level nuclear waste repository.

APPROACH

We developed a model for the Yucca Mountain unsaturated zone that represented complex heterogeneity at two different scales: (1) layer scale, corresponding to geological layering, and (2) local scale, corresponding to measurement scale. The horizontal variability of layer-scale properties was calibrated based on the available measurements collected in multiple deep boreholes. Vertical and horizontal correlation lengths were obtained using local-scale permeability and porosity data. Random fields of the three most sensitive hydrogeologic properties for a two-dimensional, vertical cross section of the site were generated by combining the average layer-scale matrix and fracture properties with local-scale perturbations (generated using a stochastic simulation method). Unsaturated water flow and conservative tracer transport were simulated throughout the cross section. The effects of multiscale heterogeneity were investigated by comparison to the homogeneous layer-wise rock properties used for mountain-scale flow and transport modeling at Yucca Mountain.

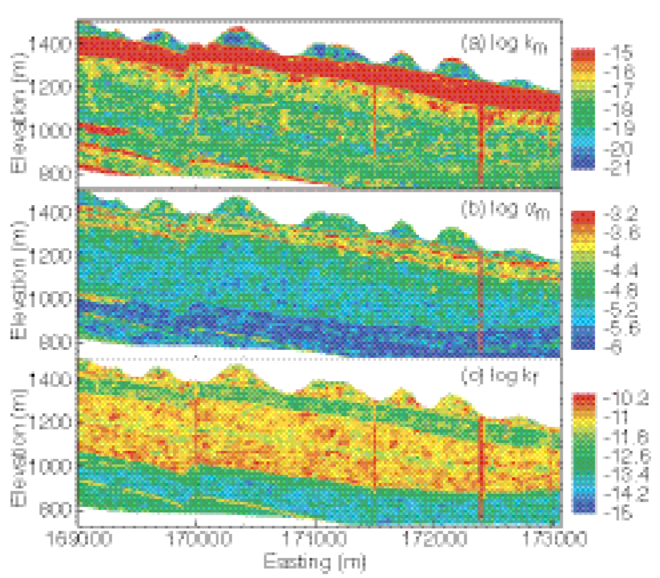

Figure 1. Random fields of matrix permeability, matrix α, and fracture permeability in the two-dimensional vertical cross section through borehole UZ-14, generated using multiscale heterogeneity

ACCOMPLISHMENTS

In addition to local-scale perturbations, the Yucca Mountain multiscale heterogeneity characterization captured the significant lateral and vertical variability in layer-scale matrix and fracture properties. This indicates that the multiscale heterogeneity of matrix and fracture properties has a considerable effect on unsaturated flow processes, leading to fast flow paths in fractures and the matrix. These paths shorten the travel time of a conservative tracer from a source (repository horizon) in the unsaturated zone to the water table. As a result, multiscale heterogeneity would seem to have a significant effect on local and global tracer-transport processes, especially for the early arrival of tracer mass. However, the effect on global transport is not significant at later times—for example, after 20% of tracer mass reaches the water table.

SIGNIFICANCE OF FINDINGS

This work has produced a useful approach for characterizing subsurface heterogeneity at different scales. It showed that multiscale heterogeneity has a significant effect on local and global flow and transport. Consequently, it improves and confirms our conceptual understanding of how rock heterogeneity affects nuclear waste disposal.

RELATED PUBLICATION

Zhou, Q., H.H. Liu, G.S. Bodvarsson, and C.M. Oldenburg, Flow and transport in unsaturated fractured rock: Effects of multiscale heterogeneity of hydrologic properties. Journal of Contaminant Hydrology, 60, 1–30, 2003.

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